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Anode Sheath Contributions in Plasma Thrusters

by

John F. Riggs Lieutenant Commander, United States Navy B.A., University of Kansas, 1982

Submitted in partial fulfillment of the requirements for the degrees of

AERONAUTICAL & ASTRONAUTICAL ENGINEER and MASTER OF SCIENCE IN ASTRONAUTICAL ENGINEERING

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13. ABSTRACT (maximum 200 words)

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Contributions of the anode to Magnetoplasmadynamic (MPD) thruster performance are considered. High energy losses at this electrode, surface erosion, and sheath/ionization effects must be controlled in designs of practical interest. Current constriction or spotting at the anode, evolving into localized surface damage and considerable throat erosion, is shown to be related to the electron temperature's ( $T_e$ ) rise above the gas temperature ( $T_o$ ). An elementary one-dimensional description of a collisional sheath which highlights the role of  $T_e$  is presented. Computations to model the one-dimensional sheath are attempted using a set of five coupled first-order, nonlinear differential equations describing the electric field, as well as the species current and number densities. For a large temperature nonequilibrium (i.e.,  $T_e >> T_o$ ), the one-dimensional approach fails to give reasonable answers and a multidimensional description is deemed necessary. Thus, anode spotting may be precipitated by the elevation of  $T_e$  among other factors. A review of transpiration cooling as a means of recouping some anode power is included. Active anode cooling via transpiration cooling would result in (1) quenching  $T_e$ , (2) adding "hot" propellant to exhaust, and (3) reducing the local electron Hall parameter. However, significant technical problems remain,

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#### I. INTRODUCTION

Several types of space flight propulsion systems have been developed over the years. These include chemical, nuclear, electric and solar propulsion. The majority of space thrusters to date have been chemical rockets. Although the Chinese used rockets over 800 years ago, true development of rocket propulsion took place during this century [Ref. 1]. Chemical thrusters give high thrust-to-weight ratios, larger than unity, and have been fully developed in the form of space launch vehicles and attitude control thrusters. In contrast, other propulsion systems have been developed only to the proof-of-concept stage, and essentially remain at this stage of development. Nuclear propulsion was studied with the NERVA (Nuclear Engine for Rocket Vehicle Application) thruster in the 1960's, and abandoned [Ref. 2:pp. 517-519]. Electric propulsion flights during the 1960's included the U.S. SERT-1 (Space Electric Rocket Test) in 1964 and the U.S.S.R. Yantari-1 rocket in 1966. Solarelectric propulsion was demonstrated via the SERT-2 rocket in 1970, powering the electric thruster from power generated by solar cells. Further electric propulsion research flights in the 1980's included the U.S. Navy's NOVA-1 satellite in 1981, and Japan's MS-T4 satellite, launched from the Space Shuttle. Beyond this, nonchemical thrusters have only been used in auxiliary roles, such as station-keeping and attitude control on geosynchronous satellites. NASA's Project PATHFINDER in the mid-1980's proposed the use of a megawatt-level electric plasma thruster for a manned Mars mission. However, development of this project was never funded.

In comparing the different propulsion schemes, a primary performance indicator is specific impulse, defined as the ratio of thrust to the rate of propellant usage, or alternately, propellant effective exhaust velocity  $(u_e)$ , divided by the sea-level gravitational constant,  $(g_o)$ .

$$I_{sp} = \frac{\dot{m} u_{\epsilon}}{\dot{m} g_{o}} = \frac{u_{\epsilon}}{g_{o}} \quad sec$$
 (1)

Chemical rockets are inherently limited in performance by the total energy available in the fuel/oxidizer combustion process, so that the total enthalpy available for conversion into exhaust kinetic energy is limited. Exhaust velocity is also limited by material heating limitations of the combustion chamber and nozzle throat, and "frozen flow Losses" (unrecoverable energy deposition in internal modes of the gas) [Ref. 3:pp. 4-5]. Peak specific impulse for liquid chemical propellants is presently on the order of 450 seconds. This capability is completely sufficient for the tasks of launch to low earth orbit (LEO), attitude control, station keeping, and such missions. However, for missions such as manned interplanetary exploration, chemical propulsion can be shown to be clearly inadequate. A comparative analysis of a Mars

mission using chemical and electric propulsion systems shows the large difference in mass payload ratio (final mass/initial launch mass) for the two systems. A chemical system using a high impulse Hohman ellipse trajectory delivers a maximum of approximately 10% to 18% of the launch mass to the Martian surface [Ref. 4:p. 115]. In comparison, an electric system using a low impulse spiral trajectory could deliver from 20% to 60% of the launch mass, depending on the desired transit time. Each mission assumes transit from low Earth orbit to Mars orbit. An electric propulsion system would still need a high thrust propulsion system to reach the Martian surface Ref. 5:pp. 344-346]. The large difference in payload ratio is due to the much larger exhaust velocity and more efficient use of fuel by electric propulsion. Thus, some form of electric or hybrid electric thruster would seem to be in order for such interplanetary missions. However, due to the low thrust-to-weight ratio of electric thrusters, they must be launched into orbit by other means. Their usefulness is restricted to space thrusters, not to launch systems.

With specific impulses of as high as 10,000 seconds, electric propulsion offers the performance envelope needed for manned interplanetary missions. Electric propulsion is divided into three types of thrusters: electrostatic, electrothermal, and electromagnetic. The type relevant to this work is the magnetoplasmadynamic (MPD) thruster, an electromagnetic propulsion system that utilizes the Lorentz force created by an electric current together with its induced magnetic field to propel a gas that has been heated to the plasma state. According to electromagnetic theory, a conductor carrying a current produces an induced magnetic force perpendicular to

the current. The applied electric field and its induced magnetic field interact to produce the Lorentz force  $(\vec{F} = \vec{j} \times \vec{B})$  perpendicular to both fields on the conductors. This briefly summarizes the concept behind the "self-field" MPD accelerator [Ref. 2:pp. 485-486]. MPD performance is enhanced by adding magnetic coils to the thruster, thus strengthening the magnetic field and, as a consequence, the Lorentz force and thrust. This thruster is appropriately called an "applied-field" MPD thruster. MPD thrusters have shown specific impulses of up to 7,000 seconds and efficiencies as high as 70% [Ref. 6:pp. 2-3]. Performance of MPD thrusters is limited by several factors, including electrode erosion, current spotting, frozen flow losses, and electrode power deposition. Specifically, anode power deposition is the single largest power loss mechanism in MPD thrusters operating at submegawatt power levels [Ref. 7]. In the following work, we review and analytically model the MPD anode, including the sheath and anode potential drop.

#### II. LITERATURE REVIEW

Anode losses significantly limit magnetoplasmadynamic (MPD) thruster performance. Much effort has been placed on characterizing these losses and on the nature of power deposition in the anode [Refs. 8-14]. As much as 80% of thruster total power may end up being deposited in the anode at sub-megawatt power levels [Refs. 8,15]. This power deposition together with current constriction at the anode surface present serious problems to thruster cooling and performance, as well as to anode lifetime. Before any practical design can be achieved, a more thorough understanding of the phenomena at the anode, particularly the anode sheath, must be gained. Studies have shown that the anode power fraction depends on thruster power, current, mass flow rate, and the parameter J<sup>2</sup>/m [Refs. 8,12,13,16]. It has also been shown that the anode fall voltage is inversely proportional to anode current density [Refs. 13,16]. It is believed that a better understanding of the role of an elevated electron temperature, of current flow dimensionality, and of current unsteadiness are prerequisites for the evolution of any practical MPD thruster design.

Computer codes that accurately describe observed data from steady-state MPD thrusters have been developed [Refs. 17-19]. However, these codes do not adequately describe observed data from quasi-steady thruster experiments. It has been suggested that the lack of proper electrode modelling (i.e., sheaths and fall potentials) in these

codes may explain this discrepancy [Ref. 6]. Limited analytical work has been done in modelling the sheath and ambipolar regions at the anode, influenced perhaps by the difficult set of coupled, nonlinear partial differential equations involved. Hugel [Ref. 12] and Subramaniam [Ref. 20] address the influence of the sheath region, but do not model the electric field, temperature, or sheath fall voltage.

Given the minuscule extent of the sheath versus thruster anode curvature, the problem at first appears one-dimensional in nature. A one-dimensional, collisional, equilibrium solution can satisfactorily reproduce the observed electric field and charge density distributions for the entire sheath and ambipolar regions for a sheath where the electron temperature equals that of the heavy species [Ref. 21]. However, this model cannot describe any decrease in current density away from the surface, or current constriction, at the anode surface which might be necessary in nonequilibrium. A two-dimensional model, developed by Biblarz and Dolson [Ref. 14], represents these phenomena and predicts the voltage drop in the region. It is shown that the sheath must account for a majority of the anode voltage drop, and that the sheath extent must be greater than the Debye length [Refs. 14,21]. Thus, a combination of one- and two-dimensional approaches appears to better describe sheath behavior. Incorporation of modelling of this sort may improve the ability of the computer codes cited above to properly describe quasi-steady thrusters.

Next, a description of the anode region is presented in order to delineate some of the possible effects of temperature.

#### III. ANODE DESCRIPTION

#### A. THRUSTER GEOMETRY DESCRIPTION

The majority of plasma thrusters to date have consisted of a central cathode rod surrounded by an annular shell anode, as shown in Figure 1 [Ref. 23]. The thruster illustrated is sufficient to produce needed thrust at current levels above one kiloamp. Below this level, an external magnetic field produced by an annular magnet is needed to ensure sufficient Lorentz force on the plasma propellant to meet thrust requirements. [Ref. 8]. As illustrated in Figure 1, the  $\vec{j} \times \vec{B}$  body force simplifies into an axial  $(j_x B_\theta)$  body force, which provides direct electromagnetic thrust ("blowing"), and a radial  $(-j_z B_\theta)$  body force, which provides electromagnetic compression of the plasma and a subsequent pressure force along the cathode surface ("pumping"). [Ref. 6]

A notable exception to this geometry is the Stationary Plasma Thruster (SPT), a design from the former Soviet Union. The SPT is an example of a plasma propulsion system known as a Hall Current Plasma accelerator. An electric field is applied axially to a stream of flowing plasma, in addition to a magnetic field with a strong radial component, which is applied by an external electromagnet. When the axial electric field is applied and a current flows through the plasma, an azimuthal component of current is induced, i.e., the "Hall" current.

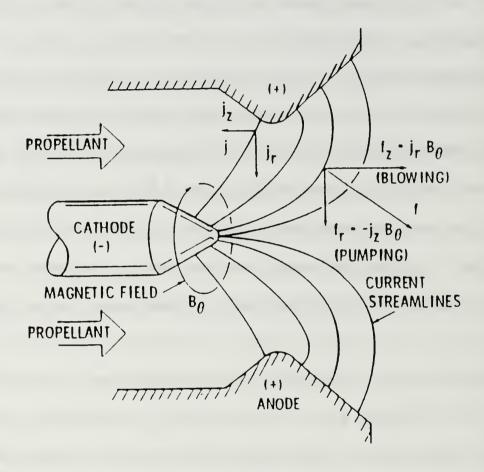


Figure 1 - Magnetoplasmadynamic (MPD) Thruster, with Axial and Radial Forces on Plasma Indicated. [Ref. 23]

Thrust is produced by electrostatically accelerating the ions in the plasma, as well as through the induced Lorentz force mentioned above. A strong radial magnetic field is applied to the plasma, whose properties are controlled to make the electron Larmor radius<sup>1</sup> small compared to the mean free path<sup>2</sup>, while the ion Larmor radius is comparatively large. As a consequence, electron mobility in the axial direction is greatly reduced. Thus, the electric field energy is given mainly to the ions, producing axial ion acceleration. Collisions with neutral particles serve to accelerate the entire neutral plasma. [Ref. 24]

A pair of the final prototype design developed, the SPT-100, have been acquired by NASA recently from Fakel Enterprise in Kaliningrad, Russia, and are undergoing performance evaluation at the Jet Propulsion Laboratory. Designed at the Kurchatov Institute of Atomic Energy (IAE) in Moscow, USSR in the 1960's, smaller versions of the SPT-100 (SPT-50 and SPT-70) were flown beginning in 1972<sup>3</sup>. A specific impulse of 1,600 seconds and 50% efficiency, as well as space flights of fifty similar thrusters is claimed. The specific operational characteristics of the thruster are not well understood presently. Bohm diffusion of electrons and a phenomenon called "near-wall conductivity" have been proposed to explain the thruster's operation. This thruster is shown in Figure 2. [Ref. 25]

<sup>&</sup>lt;sup>1</sup> Larmor radius is the radius of the helix traversed by a charged particle moving in a magnetic field.

<sup>&</sup>lt;sup>2</sup> Mean free path is the distance traveled by a particle before making a collision.

<sup>&</sup>lt;sup>3</sup>The suffix (i.e.,"-70") indicates the characteristic diameter of the thruster in millimeters.

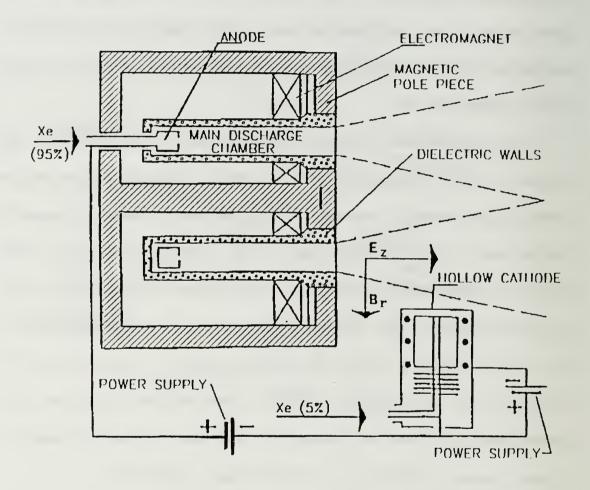


Figure 2 - Stationary Plasma Thruster [Ref. 25]

#### B. ELEMENTARY SHEATH FORMULAE DESCRIPTION

#### 1. Discussion

Voltage losses and anode power deposition account for most of the inefficiency of plasma thrusters. In order to understand these losses, the anode region must be understood and related phenomena explained and modelled. As shown in Figure 3, a substantial drop in voltage occurs in a short distance from the anode surface.

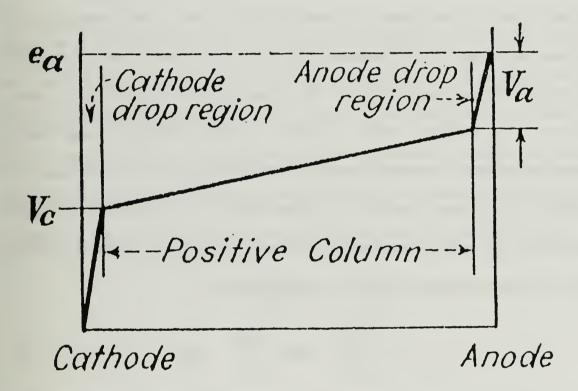


Figure 3 - Electric Field Between Two Electrodes, Including "Positive Column". [Ref. 27]

The anode fall region may be divided into two parts, the sheath and ambipolar regions. The plasma attempts to adjust itself near electrodes so as to shield the main body of the plasma from the electric field [Ref. 26]. The sheath is the region closest

to the anode surface within which the ion and electron number densities are unequal. with the electrons dominating the region. A high electron space charge exists at the anode surface. This is caused by the anode collecting incoming electrons in completing the arc current with the cathode. Positive ions are produced within the sheath by electron impact of neutral gas molecules, and the ions are repelled toward the cathode. At the cathode end of the anode drop region, the density of positive ions is high enough to almost neutralize the electron space charge, thus forming the positive column or core plasma. The essential positive ion current is created in this way near the anode. A more complete description of this process may be found in Cobine [Ref. 27] and von Engel [Ref. 28]. A fundamental characteristic of plasma behavior is its tendency toward electrical neutrality. Whenever local charge concentrations arise or external potentials are introduced into a system, these are shielded out in a distance known as the "Debye length". This distance must be much smaller than the system dimension for the ionized gas to be considered a plasma [Ref. 29]. Equation (2) gives the Debye length [Ref. 26].

$$\lambda_{\rm d} = \sqrt{\frac{\varepsilon_{\rm o}kT}{n_{\infty}e^2}} = 69.0 \sqrt{\frac{T}{n_{\infty}}}$$
 (m) (2)

<sup>&</sup>lt;sup>4</sup>The Debye length effectively describes the radius of a shell around a charged particle outside of which the potential of the particle is not seen.

Another distance of interest is the electron mean free path, or distance traveled by a particle before making a collision. Equation (3) is from a derivation of Lin, Resler, and Kantrowitz [Refs. 30,31] giving the mean free path, with  $\lambda_s$  being the approximate sheath length.

$$\lambda = 0.12 \left( \frac{1}{n_e (e^2/3kT)^2 \ln(\lambda_s e^2/3kT)} \right)$$
 (3)

Since the sheath extends at most a few mean-free lengths from the anode surface, curvature of the anode does not affect the governing equations in high pressure discharges. Thus, the region may be described in one dimension, the distance "y" from the anode surface. While the Debye length is sometimes assumed as the sheath extent, Reference 22 showed that the sheath thickness is a function of the anode fall voltage and the electron temperature. Equation (4) gives the appropriate form.

$$\lambda_{\rm s} \approx \sqrt{\frac{\epsilon_{\rm o} \Phi_{\rm a}}{e \, n_{\infty}}} = \lambda_{\rm D} \sqrt{\frac{e \, \Phi_{\rm a}}{k T_{\rm e}}}$$
 (4)

An example case with a fall voltage of 100 volts gives a sheath extent of  $\lambda_s = 2.352 \times 10^{-5} m$ . This compares to a computed Debye length of  $\lambda_D = 1.690 \times 10^{-6} m$ . Therefore, the sheath can be an order of magnitude larger than the Debye length.

13

Nasser [Ref. 32] discusses an elementary theoretical approach to the glow discharge problem. He suggests a set of four one-dimensional ordinary differential equations, including the electron and ion current and number density equations, in addition to Poisson's equation. Most solution attempts have failed, with the boundary conditions being identified as the culprit. A similar attempt for the plasma thruster is discussed below.

#### 2. Simplified Formulation

The steady probe equations are first written [Ref. 21] in their simplest form. The anode is assumed to operate as a heavily biased probe, which is true for low enough currents when the anode is not a source of ions. Whenever the temperature can be considered fixed, the energy equations are implicitly satisfied and, since ion inertia is neglected, the resulting set consists only of two species continuity equations and Poisson's equation. These equations are written in terms of y, which is the coordinate outward from the planar positive surface. Constants and variables are listed in Table 1.

## **TABLE 1 - NOMENCLATURE**

a...characteristic length of plasma n<sub>∞</sub>...species number density at core plasma

D<sub>i.e.</sub>...species diffusion coefficient N...total number density

e...elementary charge constant T...temperature

E...electric field T<sub>o</sub>...neutral species temperature

 $E_{\alpha}$ ...electric field at anode surface  $\alpha$ ...two-body recombination coefficient

 $\mathbb{E}_{\infty}$ ...electric field at core plasma  $\mathbb{E}_{\circ}$ ...permittivity constant

j<sub>i,e</sub>...species current density v...ionization coefficient

J...total current  $\mu_{i,e}$ ...species mobility coefficient

k...Boltzmann's constant  $\Phi_a$ ...anode fall potential

K...current parameter  $\lambda$ ...mean-free distance

 $n_{i,e}$ ...species number density  $\lambda_{d}$ ...Debye length

 $\dot{n}_e$ ...time rate-of-change of  $n_e$   $\lambda_s$ ...Sheath thickness

Note: Species subscripts denote ions (i) and electrons (e).

$$j_{i} = e\mu_{i}n_{i}E - (eD_{i})\frac{dn_{i}}{dy}$$
 (5)

$$j_{e} = e \mu_{e} n_{e} E + (e D_{e}) \frac{dn_{e}}{dv}$$
 (6)

$$\frac{dE}{dy} = \frac{e}{\epsilon_0} (n_i - n_{\epsilon}) \tag{7}$$

$$J = j_1 + j_2 \tag{8}$$

$$\mu_{i,e} = \frac{eD_{i,e}}{kT_{i,e}} \tag{9}$$

Here, the <u>j's are species contributions to the total current density</u>. The existence of negative charges as free electrons is pivotal in the formulation. Next, the Einstein relation, equation (9), is introduced to write the mobilities in terms of the diffusion coefficients. We assume that the diffusion coefficients remain constant in the problem.

Equations (5) and (6) are next solved for  $dn_{i,e}/dy$ . The species current density equations are found from the net reaction rate of the plasma. Equations (10) and (11) combine to produce space derivatives for species current density.

$$\dot{n}_e = v_i n_e - \alpha n_i n_e \tag{10}$$

$$\frac{d\dot{j}_{i}}{dv} = \frac{-d\dot{j}_{e}}{dv} = e\dot{n}_{e} \tag{11}$$

Combining equations (5)-(11) produces a set of five coupled, non-linear differential equations describing the sheath. These are nondimensionalized to adjust all variables to the first order, and are rewritten below as equations (12)-(16), with nondimensionalized variables denoted by "x̄". Nondimensionalization can be accomplished as follows: The species number densities nend, are divided by their values at infinity to produce output from the anode surface to unity at the ambipolar boundary. The current densities je,je are divided by the total current, allowing the output to show the "mirror behavior" of the two currents. The electric field is divided by the initial anode value to give output starting from unity at the surface and decreasing to the final core field value. The variable "y" is divided by the characteristic length of the plasma, "a", producing ŷ. These corrections allow all output to vary in the range from zero to one, as a function of distance from the anode.

<sup>&</sup>lt;sup>5</sup>The characteristic length is defined so as to cancel the multiplying factor in the electric field equation, (14), ( $a = 1.107 \times 10^{-6}$ ). This allows a physical interpretation of the ion/electron number densities, as well as the decay rate of the electric field.

$$\frac{d\tilde{n}_{i}}{d\tilde{y}} = \left(\frac{aeE_{o}}{kT_{o}}\right)\tilde{n}_{i}\tilde{E} - \left(\frac{aeE_{\infty}}{kT_{o}}\right)\tilde{j}_{i}$$
(12)

$$\frac{d\tilde{n}_{\epsilon}}{d\tilde{y}} = -\left(\frac{aeE_{o}}{kT_{o}}\right)\tilde{n}_{\epsilon}\tilde{E} + \left(\frac{aeE_{\infty}}{kT_{o}}\right)\tilde{j}_{\epsilon}$$
(13)

$$\frac{d\tilde{E}}{d\tilde{y}} = \left(\frac{\operatorname{aen}_{\infty}}{E_{\circ}\epsilon_{\circ}}\right) (\tilde{n}_{,} - \tilde{n}_{\epsilon})$$
 (14)

$$\frac{d\tilde{j}_{e}}{d\tilde{y}} = -\left(\frac{akT_{o}v_{i}}{eE_{\infty}D_{e}}\right)\tilde{n}_{e} (\tilde{v}_{i}-\alpha\tilde{n}_{i})$$
(15)

$$\frac{d\tilde{j}}{d\tilde{y}} = \left(\frac{akT_o v_i}{eE_{\infty}D_e}\right) \tilde{n}_e \left(\tilde{v}_i - \alpha \tilde{n}_i\right)$$
 (16)

Attempts to solve this equation set using the computer code discussed below shows the set to be extremely sensitive to initial conditions. The computer code solver uses a "marching" scheme from the anode to the undisturbed plasma. The initial conditions are chosen to produce the electric field potential drop observed in actual thrusters. First and second space derivatives of the electric field are used as diagnostic checks to ensure reasonable output values and indicate instability of the integration process. Figure 4 shows the required resulting curves for the electric field and its first and second derivatives.

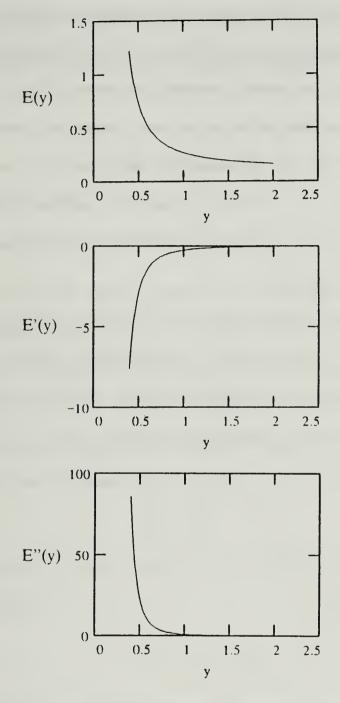


Figure 4 - Electric Field and First Two Space Derivatives Used as Diagnostic Checks for Integrator Output. (Plotted for a Generic Exponential Function).

Ecker characterizes the plasma at the anode as a double sheath, with the inner section called the "inertia sheath", and an outer section called the "energy loss section". The inner section shows a potential rise of the order of one volt, with the outer section showing the exponential potential drop shown in Figure 4. While this double sheath may in fact describe the actual sheath region, the formulation above only models the potential drop portion of the sheath, and does not attempt to produce the potential rise of the inner sheath. In addition, Ecker's current constrictions are of a "macroscopic" nature, whereas those of Reference 14 and this work are "microscopic" [Ref. 33].

Data for a 6,000°K Nitrogen plasma were used to test the equation set [Ref. 21]. Producing a proper solution required adjusting the initial conditions to force the curve shapes discussed above. Using Equations (2), (3), and (4), the mean free path, Debye length, and approximate sheath extent are calculated as  $\lambda = 9.352 \times 10^{-3}$  m,  $\lambda_D = 1.690 \times 10^{-6}$  m, and  $\lambda_S = 2.352 \times 10^{-5}$  m (this assumes a drop voltage of 100 volts).

#### 3. Approximate Formulation

Reference 21 explores the above equation set by taking advantage of the symmetry among the equations, and introducing two parameters, K<sup>+</sup> and K<sup>-</sup>, shown below.

$$K^* \equiv \frac{j_i}{e D_i} + \frac{j_e}{e D_e} \tag{17}$$

$$-K^{-} \equiv \frac{j_{i}}{e D_{i}} - \frac{j_{e}}{e D_{e}}$$
 (18)

It can be shown that the resulting equations can be manipulated to yield a single, ordinary differential equation for the K's in terms of the electric field. The resulting equation can be scrutinized for two distinct temperature regimes. Note that while the total current density, J, is constant in a steady, one-dimensional case, the K's can vary and will in turn also depend on the degree of reactivity of the plasma ( $\dot{n}_e$ ), i.e.,

$$\frac{dj_i}{dy} = \frac{-dj_e}{dy} = e\,\dot{n}_e \tag{19}$$

Because ion diffusion is much slower than electron diffusion, it can be shown that the K's are related by

$$K^- \approx -K^- + \frac{2J}{eD_e}$$
 (20)

As will be evident, at the electrode surface the K's are equal to each other and at the undisturbed plasma,  $K^- = 0$ . The total current density may be evaluated from

$$J = e n_{r} v_{r} \tag{21}$$

where  $v_{ex}$  is the electron drift velocity beyond the ambipolar region which is strictly a function of  $E_x/N$ , (i.e., of the ratio of undisturbed electric field to the total number density).

### a. Effects of Temperature on Anode Constriction

It is useful to investigate the overall effects of temperature. Since temperature will be considered constant, it comes in as a parameter in this formulation whereas charge density and electric field remain as variables. Intuitive arguments will be introduced which suggest that the electron and ion/neutral temperatures play a rather singular role in determining the intrinsic dimensionality of the problem, (i.e., there are cases when the geometry of the current lines is not necessarily impressed by the electrode geometry). Since the problem is described by moderate pressure, largely collisional sheaths, the ion and neutral temperatures are anticipated to remain reasonably equal. Depending on the gas, the electron temperature, on the other hand, can be elevated from the gas temperature at the anode where actual magnitudes depend on the local value of E/N. In order to get a perspective on the effects of temperature, we shall consider two extremes, namely, the case where the electron and ion temperature are the same (the equilibrium case) and the case where the electron temperature is substantially elevated from that of the ions/neutrals (the two-temperature case).

(1) Case I: 
$$T_e = T_i = T_o$$
 (Equilibrium)

The charge densities can be eliminated by combining equations (5)-(9), (17) and (18). The resulting equation can be shown to be

$$\frac{kT_{o}}{e} \left(\frac{K^{*}}{E}\right)' + K^{*} = \frac{2J}{eD_{e}} - \left(\frac{kT_{o}\epsilon_{o}}{e^{2}}\right) \frac{1}{E^{2}} \left[EE'' - (E')^{2} - \frac{1}{4}(\frac{e}{kT_{o}})^{2}E^{4}\right]'$$
(22)

If the electric field decreases monotonically from the wall to the undisturbed plasma (i.e., from  $E_o \to E_\infty$ ), then as  $y \to \infty$ ,  $E \to E_\infty$ ,  $E' \to 0$ ,  $E'' \to 0$ .

So that in equation (22) above the "outer solution" becomes:

$$K^{-} = \frac{2J}{eD_{c}} \tag{23}$$

Now this represents an acceptable solution from a physical point of view. Moreover, as  $y \to \infty$ ,

$$\dot{\mathbf{n}}_{\bullet\bullet} \approx \mathbf{D}_{\bullet}(\mathbf{K}^{\bullet})' \approx 0 \tag{24}$$

which is also acceptable for an equilibrium situation at the undisturbed plasma. Results [Ref. 21] are shown in Figure 5 for the case of nitrogen at 6000°K using an approximate electric field distribution.

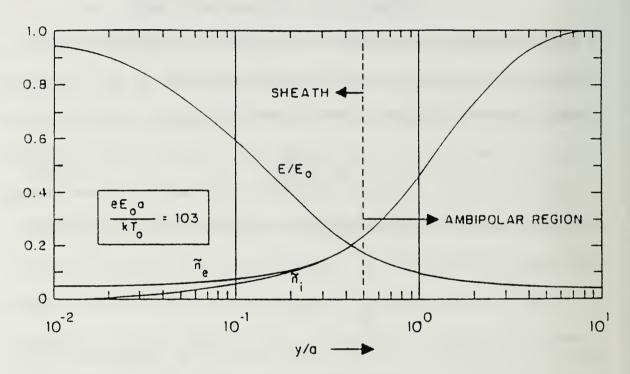


Figure 5 - Electric Field and Species as a Function of  $\tilde{y}$ , Distance From Anode. An Approximation Using a Shaped Electric Field and Isothermal Plasma [Ref. 21].

# (2) Case II: $T_e >> T_i = T_o$ (Two-Temperature)

In this case the same procedure as before yields the following equation where terms divided by  $T_e$  have been dropped when compared to their counterparts divided by  $T_o$ .

$$(K^{*})' - \frac{K^{*}}{E} E' = \frac{2EJ}{kT_{o}D_{e}} + \frac{2\epsilon_{o}}{kT_{o}} EE'' + \frac{\epsilon_{o}}{eE}E''E' - \frac{\epsilon_{o}}{e}E'''$$
 (25)

Assuming the same monotonic decrease as before for the electric field from the wall to the plasma proper, as  $y \to \infty$ ,  $E \to E_{\infty}$ ,  $E' \to 0$ ,  $E'' \to 0$ .

Then the outer solution becomes

$$\frac{dK^*}{dy} \approx \frac{2eEJ}{kT_0eD_e} \quad \text{with } \dot{n}_{e\omega} > 0$$
 (26)

Or,  $K^* \rightarrow$  (constant) y + constant, and  $\dot{n}_{e^{\infty}}$  keeps increasing with y.

This is <u>not</u> the proper outer solution for the one-dimensional, equilibrium plasma that we seek because the net ionization rate continues to increase well inside the plasma proper where conditions should saturate, yielding a constant electric field. Therefore, as formulated, Case II is not amenable to a one-dimensional solution. References 14 and 21 show how this case can be analyzed under a multidimensional approach. These references also discuss a method for describing the electron temperature as a function of E/N, then how to couple a simplified energy relation which satisfactorily describes a two-temperature plasma. The necessary ingredient to make equation (26) approach zero beyond the decrease of E to E<sub>x</sub> is to allow J

to fan out as indicated in Figure 6. Thus, in equation (26), the product "EJ" can bring down the charge production rate to arbitrarily low values. Alternatively, it is possible to explore techniques of bringing the electron temperature down to be in closer equilibrium with the ions and neutrals. Transpiration cooling is one such means.

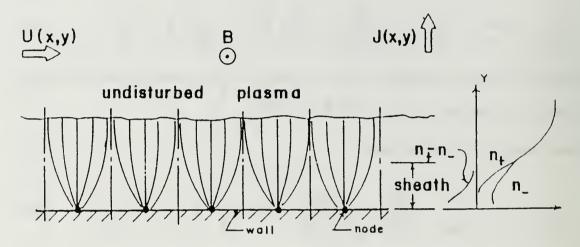


Figure 6 - Two-Dimensional Model of Current Paths Showing Periodic Structure. Thermal Instabilities and Inhomogeneities Would Favor One Site Over Others and a Single Macroscopic Constriction May Then Be Produced. [Refs. 14, 34]

### b. Similarity to Vacuum Arc Phenomena

Instability phenomena observed in vacuum arcs [Ref. 35] are very similar to those observed in self-field thrusters [Ref. 12]. After the establishment of the current, the anode region operates in a vapor that issues from the electrodes. In vacuum arcs, Miller characterizes the anode region as operating in one of five distinct modes, ranging from a passive, low current mode to a high current, fully developed spot mode [Ref. 36]. Given the similarities mentioned above, vacuum arc anode research should be helpful in the understanding of MPD thruster transition to the anode spot mode. Existence diagrams after Miller [Ref. 36] are shown in Figure 7, which divide operating modes into regions as a function of anode current versus electrode geometry. Figure 7 shows the transition from glow to spot mode.

Anode spot formation at high currents is clearly a factor in limiting anode lifetime. Various phenomena have been related to anode spotting. Hugel [Ref. 12] relates the transition to spotting mode to an increase in J²/m above a critical level. A separate factor connected with the spot mode is surface temperature of the anode. Rich, et.al., [Ref. 37] show that anode spotting is preceded by a luminous "footpoint" and followed by local melting prior to spot formation. Separately, Schuocker [Ref. 38] finds a connection between spotting initiation and the factors of anode evaporation and magnetic constriction in vacuum arcs with high currents. Experimental investigations must be performed to see if the above-mentioned vacuum arc criteria apply to self-field thrusters.

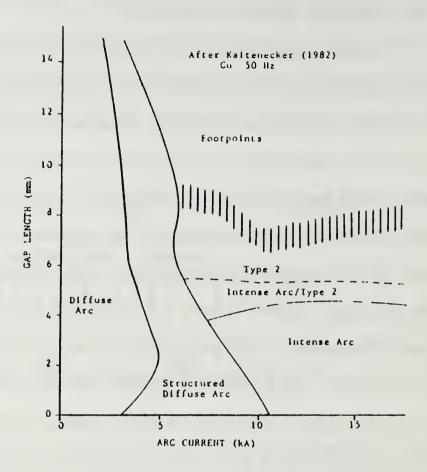


Figure 7 - Anode Discharge Modes as a Function of Current and Gap Length. [Ref. 36]

### C. COMPUTER CODE

Rather than using linear approximations to equations (12)-(16), the nonlinear set was used, with initial conditions adjusted in an attempt to produce observed electric fields from probe data. First and second space derivatives of the electric field were used as diagnostic checks to ensure computed output was reasonable. Initial conditions computed from the approximate formulae in Reference 21 were used. The equation set above presents a difficult problem for two reasons, nonlinearity and multiple time constants. The species number density equations, (12) and (13), both contain a nonlinear term, each with a time constant of its own. In addition, the electric field equation, (14), adds a possible third time constant. This constitutes a "stiff" set of equations. Attempts were made to solve the set with the data discussed above, using Gear's method of backward differentiation, in hopes that the variables would change slowly enough with each iteration to render a convergent iterative process. As described in Reference 39, if some reactions are slow and others fast among a set of coupled equations, the fast ones will control the stability of the method. This is addressed in the DGEAR program available from the International Mathematical & Statistical Library (IMSL). The latter software contains an Adams predictor-corrector method, as well as Gear's method, which is well known for its success at solving stiff equation sets. The DGEAR software allows for a choice of functional or chord iteration methods, as well as a choice of Jacobian matrices. A more detailed discussion of this software can be found in Reference 39 and in the IMSL library. [Ref. 39]

#### D. COMPUTATIONAL RESULTS

Numerous computer runs were completed using the initial conditions taken from Reference 21. In addition, data for the ionization coefficient v, Figure 8, was taken from References 40 and 41.

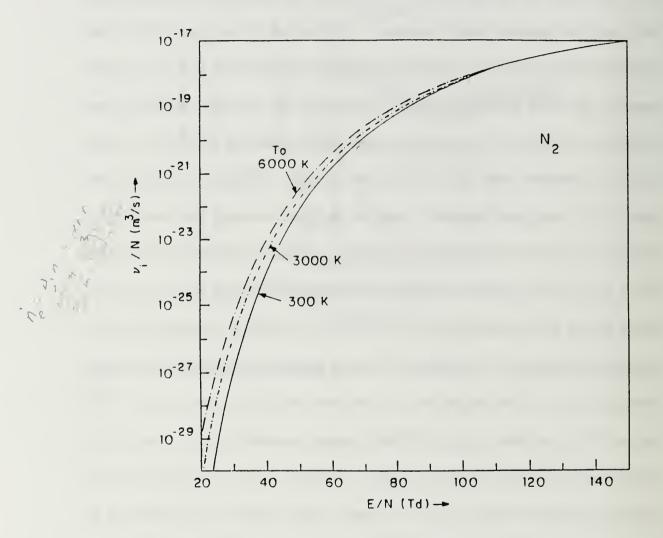


Figure 8. Ionization Coefficient v as a Function of E/N for Nitrogen for Various Vibrational Temperatures (Refs. 40,41).

Various combinations of initial conditions and ionization coefficient were used. As mentioned above, the electric field and its space derivatives were used as diagnostic/reasonability checks on the output. Individual, as well as multiple computer runs were attempted to model the sheath region. Nonlinearities in the equation set are clearly seen in Figure 9. The ion number density does not reach that of the electrons, and the latter population growth rate continues to grow without bound. The shape of the electron population curve is very sensitive to its initial value. As shown in Figure 9, the latter population has too high a growth rate when compared to the ion population, and the latter does not "catch up". Increasing the initial value of  $\tilde{n}_e$  flattens out this curve to a reasonable shape. Above an initial value of approximately 0.06, however, the plot of  $\tilde{n}_e$  "dips" after a certain distance and then continues to increase as expected. This gives an approximate upper value for this initial value. To avoid instabilities like this, small "slices" were taken of the output after a small number of integration steps and multiple runs were used to form a "cut and paste" plot of the region. When a reasonable plot shape was produced, the value of ionization coefficient was varied in the "slices" to attempt to produce the required end values for electric field and species population. Both multiple and equilibrium values for the ionization coefficient were used. When the data showed signs of instability and failure to follow the required forms of Figure 4, a "slice" was made in the data stream, and the data points from this point used to start a new computer run. This approach was taken in the hope of avoiding singularities in the integration from anode surface to ambipolar region. In addition to the diagnostic checks shown in Figure 4, an additional data check is provided by the transition from the sheath to the ambipolar region.

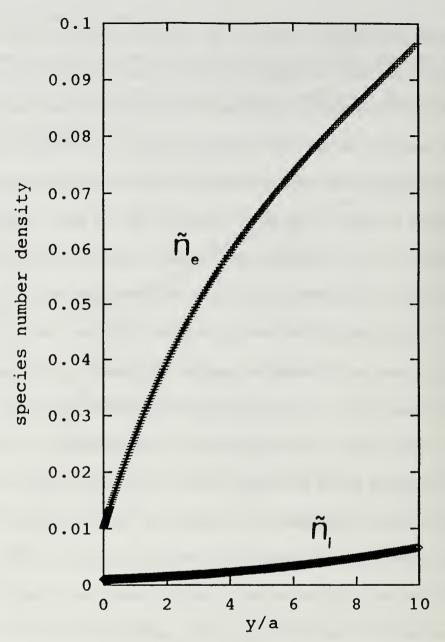


Figure 9. Species Number Density plots for Individual Computer Run, Showing Divergent Tracks for Ion and Electron Populations, and Effect of Nonlinearity.

As shown in Figure 5, the species number densities are equivalent in this region, as are their change rate. Thus, setting Equations (12) and (15) equal to each other and solving for ñ yields a value of 0.5 in the ambipolar region. As indicated in Figures

10-11, the output produces the desired plot slopes for electric field and species number density. However, the number density plots cross long before approaching the required value of 0.5. In addition, neither electric field nor species number density approaches an equilibrium value or shows sign of levelling off. Apparently, the multiple time constants and nonlinear portions of the number density equations combine to create a seemingly intractable system. Solutions for this system may be possible for specific, individual initial condition sets, but the problem does not appear amenable to this approach in general. A one-dimensional system such as this may be better described through the approach of boundary layer theory or nonlinear dynamics and chaos. Given the effort and difficulty involved in the latter, a onedimensional approach such as that modelled above does not appear useful. A combination of one- and two-dimensional modelling would appear to be more useful, as discussed in Reference 14. A one-dimensional model may be useful, but only in an approximation approach, with a shaped electric field, such as that used in Reference 21.

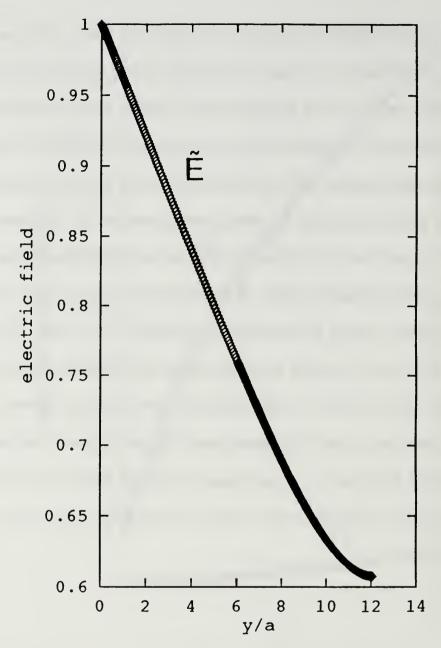


Figure 10. Electric Field as a Function of  $\tilde{y}$ , Distance From Anode, Using Equations (12)-(16).

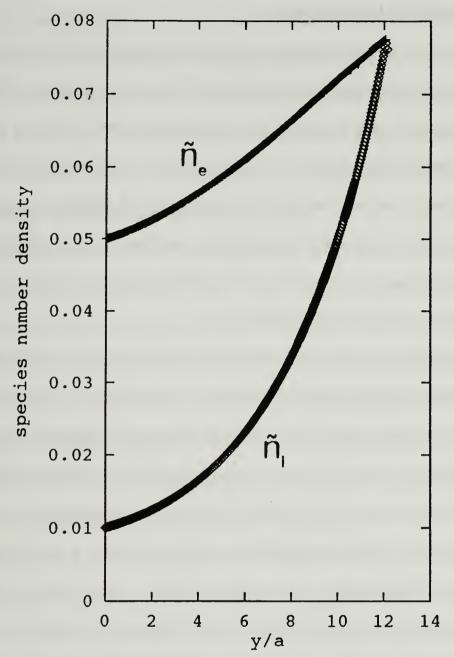


Figure 11. Species Number Density as a Function of  $\tilde{y}$ , Distance From Anode, Using Equations (12)-(16).

### E. ANODE FALL VOLTAGE

The arc discharge operates with an anode voltage drop ( $V_{af}$ ) which should be on the order of the ionization potential of the gas as it is in glow discharges. This voltage drop is largely non-ohmic because the anode region is typically very thin and space-charge controlled. Since a significant portion of the anode heating comes via the oncoming electrons accelerating through the fall voltage, it is of interest to minimize this voltage, which can range from less than ten to over 40 volts in argon. The question arises as to what governs this anode drop and why is it such a noticeable function of current? [Ref. 42]

In collisional sheaths, the anode voltage drop is largely governed by a positive ion generation region which forms in front of the anode. The production of ions reduces the space charge density and thereby permits operation at lower voltages than otherwise possible. Ions are most often created by electrons within their last few mean-free-paths before entering the anode; these ions slowly drift away from the anode, thereby effectively neutralizing the space charge, at a speed proportional to the ratio of their mobility to that of the electrons. At the anode, the electric field is a maximum and the electron mean energy displays a corresponding high.

At moderate pressures, the sheath is very thin and breakdown can be visualized as occurring between the undisturbed plasma (which acts as a rich source of electrons) and the anode surface. This arrangement has the attributes that represent "thermionic arc breakdown" [Ref. 43], a source of electrons which is independent of the breakdown itself and relatively small spacings. For gases that allow cumulative

ionization (with some help from the tail of the Maxwellian distribution of electron energies), what results is a breakdown voltage appreciably below the ionization potential. This then could be an explanation for the low voltage breakdown observations [Ref. 42]. Clearly, gases with low ionization potentials and lots of atomic electron energy levels are preferred (such as cesium and barium) but low-voltage breakdown has been observed with most gases.

The increase of the anode fall voltage above the ionization potential has been related to the electron Hall parameter, since a reduction of this parameter decreases that voltage and corresponding losses. Control of the local magnetic field through the use of and array of permanent magnets as well as implementation of transpiration cooling (which increases the electron collision frequency) have both yielded some encouraging results. Because the anode fall also scales up with  $J^2/\dot{m}$ , it is conceivable that current inhomogeneities and plasma instabilities which are reflected in this parameter are in the picture as well. [Ref. 44]

In summary, any possible reduction of the anode fall voltage will hinge on a thorough understanding of the anode region, with its associated sheath and ambipolar regions, where electron temperature effects, ionization effects, and magnetic field effects play a pivotal role. If transpiration cooling is present, then additional phenomena of fluid-dynamic nature may come into play. Experimental observations with atmospheric discharges indicate the possible presence of convective effects at the anode. [Ref. 45]

### IV. TRANSPIRATION COOLING

Transpiration cooling of the anode has often been promoted as an attractive means of recovering a large portion of the power deposited there. Additionally, the onset of melting may be minimized or even avoided by active anode cooling. Rich, et.al., related high anode temperatures to anode spotting [Ref. 37]. Similarly, Park and Choi showed that low thermal diffusion leads to erosion and, consequently, anode damage [Ref. 46]. Active anode cooling via transpiration is one means of ensuring high thermal diffusion and extending anode lifetime. Early work by Schoeck, et. al., [Ref. 47] showed that up to 80% of the energy deposited in the anode is recoverable via transpiration cooling. While this study used non-convective, high-intensity argon arcs, it is reasonable to assume that this effect would apply in MPD arcs using other propellants. Although this cooling method has not been studied for incorporation in plasma thrusters for some time, it has been recently considered as a means of cooling the fuselage of the National Aerospace Plane (NASP). Plasma thruster designs could undoubtedly gain from this database, and due consideration should be given to this cooling approach for the anode.

For a given mass transfer flow rate, the heat flux reduction to a surface is inversely proportional to the molecular weight of the injected gas. Use of the propellant as coolant as well as fuel would eliminate the need for additional tankage and pumps, simplifying the design considerably. Lithium has been considered to be

the propellant of choice, primarily because of its low molecular weight, its favorable ionization potential, and its low-volume tankage properties. It has a relatively low first ionization potential of 5.4 eV and a high second ionization potential of 75.6 eV. This single ionization potential range of over 70 eV compares to approximately 20 eV for Cesium and 27 eV for Potassium [Ref. 48]. This provides a broad temperature range within which only single ionization will occur. Large temperatures must be reached within the gas before double ionization occurs. As the gas temperature is increased several thousand degrees Kelvin, it undergoes ionization and disassociation. Thermal energy deposited can be recovered through nozzle expansion at the exit. However, residence time of the gas is not long enough to ensure recombination. Thus, the energy invested in ionization and disassociation will be lost. [Ref. 49] Lithium has been shown to produce specific impulse figures in excess of 7,000 seconds at 70% efficiency in steady-state thrusters, [Ref. 50] whereas all other propellants have been limited to less than 3,000 seconds specific impulse at less than 40% efficiency [Ref. 6]. Subramaniam has concluded that:

...regenerative cooling of anodes (at the specific impulse values in the MPD regime) is possible only with hydrogen or with alkali-metal propellants, notably lithium. In the latter case, the ideal anode operating mode would be evaporation and ionization of the propellant on the porous or wetted anode surface, resulting in increased ion current fraction, reduced anode voltage fall and utilization of part of the anode loss energy [Ref. 51].

Liquid coolants, as well as reducing storage requirements, offer the advantage of providing latent heat of vaporization for energy disposal. However, design problems can occur if the liquid is allowed to vaporize within the porous structure. Problems

arise due to the abrupt increase in pressure gradient as the coolant vaporizes. Since coolant flow generally have three-dimensional characteristics, the flow will be diverted around the vapor bubbles and hot spots often develop. The technical practicality of using molten lithium to cool a porous tungsten anode would seem to be beyond current technology. On the other hand, the products of decomposition of hydrazine (gaseous hydrogen and ammonia) have proven to be efficient and practical coolants [Ref. 52].

Given the performance figures above, using an auxiliary coolant gas even with high molecular weight (e.g., NH<sub>3</sub>, N<sub>2</sub>, CH<sub>4</sub>, etc.) which could serve as a propellant once released from a porous hot tungsten anode surface would seem to more practical, vice dealing with molten lithium. Experimental studies would be needed to compare the approaches. Kuriki and Suzuki performed experiments with a quasisteady MPD thruster to study the effect of anode gas injection (Argon). At high currents of up to 10 kA, increases in thrust, specific impulse, and flow discharge stability were observed [Ref. 53].

There is some question as to the likelihood of current constriction <u>resulting</u> from anode gas injection. In such a case, swirling or circulating the propellant gas would help to move any footpoints that developed around the anode surface and prevent them from becoming fully-developed spots. Additionally, an applied magnetic field could serve to circulate the footpoints as well. The unique advantage of transpiration cooling hinges on providing effective anode cooling while supplying

hot propellant, but the real benefit will depend on how small the amount of coolant required really will be.

Transpiration cooling has proven to be as desirable as it is challenging. It is complicated to implement, with associated reliability problems and difficulty of analytical predictions. While the production of thicker boundary layers is largely ineffective against the electron flux heating, the cooling itself is most efficient and a substantial fraction of the energy transferred to the anode is recoverable. The arguments of Chapter Three indicate that a reduction of the electron temperature in the anode would have the desirable effect of reducing the initial current spotting which can be conjectured to be the path that leads to anode arc spots. This electron temperature reduction can be done most effectively by polyatomic gases (which have a high  $\delta$ -loss factor) emanating from the anode surface [Ref. 54].

The arguments relating to transpiration cooling might be summarized as follows:

## Favorable Outcomes

- · No separate cooling mechanism for anode required,
- Adds "hot" propellant to exhaust "recovering" most of the electrical power loss to the anode,
- Quenches T<sub>e</sub> thus likely to postpone anode spotting <u>and</u> reduce the heating associated with the electron thermal energy (5kT<sub>e</sub>/2e),
- · Reduces bulk convective heating,
- · Reduces the local electron Hall parameter by increasing the collision frequency,

### Favorable Outcomes (cont'd.)

- Allows for some radiation cooling from the hot tungsten surface (about 120 watts/cm² at 2800°K [Ref. 51]),
- Hydrogen/ammonia gases flowing through hot porous (sintered) tungsten represent a compatible, proven technology.

### Unfavorable Outcomes

- · May decrease the electrical conductivity in the anode region,
- May destabilize the ionization processes in the sheath and bring about significant fluctuations in the current,
- · Disrupts "cathode jet" in front of the anode with unpredictable consequences,
- Introduces propellant which may not be hot enough, not ionized enough, or not in the proper place for  $\vec{j} \times \vec{B}$  acceleration,
- Transpiration cooling through a porous (tungsten) anode is a difficult design problem.

### V. CONCLUSIONS AND RECOMMENDATIONS

Plasma thrusters offer distinct advantages in terms of payload delivered for interplanetary missions, as well as for orbital transfer. A recent comparison completed by Choueiri, Kelly, and Jahn shows a mass savings of 65 tons for an orbital transfer from low Earth orbit to geosynchronous Earth orbit using a quasisteady MPD thruster as opposed to an advanced chemical thruster. This superior performance comes at the expense of low thrust-to-weight ratio and long transit time. However, given the large cargo/logistic requirements of a manned interplanetary mission, delivery of payload must be maximized. Thus, further work to characterize more fully thruster behavior and anode contributions in particular are certainly warranted. [Ref. 55]

The "cut-and-paste" method used to generate Figures 10 and 11 is not of practical use as a modelling method, due to the large effort involved. It did produce the expected electric field and species number and current density plots near the anode, but failed to produce the entire sheath out to the ambipolar region. The nonlinearity of the equation set led to a quickly deteriorating solution. A more practical approach using nonlinear dynamics and/or chaos must be developed to model the sheath numerically.

This assumes a specific impulse of 2,000 seconds, 600 kW of input power, and a 270-day transit time.

Depending on the propellant mass fraction used for cooling, the transpiration scheme discussed above presents some rather unique advantages. A hot anode which uses only a small amount of propellant for cooling need not be penalized for any lost thrust. If in addition, we increase anode lifetime by delaying the formation of anode arc spots, then the scheme is all the more desirable. A decrease of the electron temperature in the vicinity of the anode may bring about a more homogeneous flow of current and a reduction in the heating effect associated with the high electron kinetic energy. Recovery of the heat deposited at the anode would be most important if the propellant fraction is high. In such case, nozzle expansion of the hot-propellant/coolant-gas might be implemented.

Means of limiting anode losses through decreasing anode fall voltages were discussed, including the control of the local Hall parameter and the implementation of thermionic arc breakdown. The electrical conductivity (of a nonreacting plasma) could possibly decrease as a result of transpiration cooling and this might increase the anode fall voltage.

Additional work needs to be done in the following areas:

- Investigate effectiveness of nonlinear dynamics and chaos in solving sheath equation set,
- Incorporate adequate one- or two-dimensional sheath modelling in quasisteady

  MPD numerical codes,

- Investigate the role that fluid dynamic effects play in MPD thruster anode discharges,
- Investigate the effect of transpiration cooling on current and plasma stability, as well as on thruster performance and lifetime,
- Determine effectiveness of transpiration cooling's increase of the collision frequency parameter,
- Compare performance of gaseous propellant/coolants versus hybrid designs with lithium propellant/gaseous coolant,
- Determine if required percentage of propellant gas as coolant is practical (e.g., less than 10%),
- Investigate effect of surface imperfections as focal points for current constrictions and as precursors to anode spotting.

#### APPENDIX A

The following software includes the calling program, SHEATH, its two subroutines, FCNJ and YDOT, and the DGEAR integrator. The latter is quite extensive in length and includes ten subroutines, including the following: DGRST, DGRCS, DGRPS, DGRIN, LUDATF, LUELMF, LEQTIB, UERTST, UGETIO, and USPKD. A detailed discussion may be found in IMSL literature or Reference 39.

```
*******************
     Program Sheath
                                                                          000010
C
                                                                          000020
C-----Calling program for DGEAR integrator. Initial conditions are
                                                                          000030
     input via READ statements and keyboard entry. Output is to data
С
                                                                        000040
С
     files via the DGRST subroutine. Diagnostic check of output via
                                                                          000050
     Figure 4 printed to data file from DGRST subroutine. Consult
С
                                                                         000060
С
     DGEAR comments for variable descriptions not listed below.
                                                                          000061
C-----
                                                                          000062
     REAL E, K, EPS, TI, EF, EFINF, DI, DE, NUINF, C1, K1, A
                                                                         000070
      INTEGER N, METH, MITER, INDEX, IWK(1), IER, STEP
                                                                          000080
      REAL*8 X, H, Y(5), XEND, TOL, WK
                                                                          000090
      EXTERNAL YDOT, FCNJ, DGEAR
                                                                          000100
      COMMON/CONST/E, K, EPS, TI, EF, EFINF, NINF, DI, DE, VINF, C1, K1, A
                                                                          000110
C
                                                                          000120
C------Constants
                                                                          000121
С
     C1 and K1 are constants describing the ionization coefficient.
                                                                          000122
С
    They are taken from the data plotted in Figure 8. The
                                                                          000123
     coefficient is equal to the nondimensionalized electric potential 000124
С
С
     raised to the K1 power and then multiplied by C1.
                                                                          000125
С
     In this way, the ionization coefficient is allowed to vary in
                                                                         000126
C
     proportion to the strength of the electric potential.
                                                                          000127
C-
                                                                          000128
      WRITE(*,*)'Input value for C1 (format 6E3):'
                                                                          000129
      READ (*,*) C1
                                                                          000130
      WRITE (*, *) C1
                                                                          000131
      WRITE(*,*)'Input value for K1 (format 6E3):'
                                                                          000132
      READ (*, *) K1
                                                                          000133
      WRITE(*,*)K1
                                                                          000134
      Initial conditions for species number density, electric potential 000135
C
C
     and species current density are now input (ni,ne,E,je,ji).
                                                                          000136
C----
                                                                          000137
      WRITE(*,*)'Input values for y(1) through y(5) (format 5(6E3)):'
                                                                          000138
      READ (*, *) y (1), y (2), y (3), y (4), y (5)
                                                                          000139
      WRITE (*, *)y(1), y(2), y(3), y(4), y(5)
                                                                          000140
      Following constants are for plasma described in Reference 21
С
                                                                          000141
C
      (6,000 \text{ K}, \text{ Init } E=20,000 \text{ V/m}, \text{ Final } E=1,200 \text{ V/m})
                                                                          000142
                                                                          000143
      E=1.6E-19
      K=1.38E-23
                                                                          000150
                                                                          000160
      EPS=8.854E-12
      TI=6E3
                                                                          000170
      EF=2E5
                                                                          000180
                                                                          000190
      EFINF=1.2E4
                                                                          000200
      DI=1.724E-4
      DE=1.724E-1
                                                                          000210
                                                                          000215
      VIO = 2.E6
      VINF = 4.93E-7
                                                                          000220
C
                                                                          000230
```

```
A is plasma characteristic length which shows potential drop.
C
                                                                          000240
      A = ((EPS*EF) / (E*NINF)) = 1.107E-6
C
                                                                         000250
      A = 1.107E-5
                                                                          000270
      X = 0.01
                                                                          000280
      XEND = 10.
                                                                          000290
      H = 1e-6
                                                                          000300
      TOL = 1E-6
                                                                          000305
      METH = 2
                                                                          000310
      MITER = 1
      INDEX = 1
                                                                          000320
                                                                          000330
      N=5
                                                                          000340
      IWK(1) = 5
                                                                          000350
      WK = 18000.
                                                                          000360
      IER = 0
      OPEN (UNIT=8, FILE='SHEATH.DAT', STATUS='UNKNOWN')
                                                                          000370
                                                                          000380
      CALL DGEAR2 (N, YDOT, FCNJ, X, H, Y, XEND, TOL, METH, MITER, INDEX, IWK, WK,
                                                                          000390
     +IER, STEP)
                                                                          000400
      DO 3 I=0, N
                                                                          000410
   DO 2 J=0,100
      WRITE (*, *) J, Y(I)
                                                                          000420
                                                                          000430
      WRITE(8,1)J,Y(I)
      FORMAT (T2, F5.1, 5 (5X, D9.2))
                                                                          000440
  1
                                                                          000450
  2
        CONTINUE
                                                                          000460
      CONTINUE
  3
                                                                          000470
      WRITE(*,*)'Total Steps = ',STEP,'Final Step Size = ',H,
     +'Error Code = ',IER
                                                                          000480
                                                                          000490
      CLOSE (UNIT=8)
                                                                          000500
      STOP
                                                                          000510
      END
C*********
C DUMMY SUBROUTINE FCNJ
C*********
      SUBROUTINE FCNJ (N, X, Y, PD)
                                                                               1
                                                                                2
      INTEGER N
                                                                               3
      REAL Y(N), PD(N, N), X
                                                                               4
      RETURN
                                                                                5
C**********
C SUBROUTINE YDOT
C*********
      SUBROUTINE YDOT (N, X, Y, YPRIME, eprime, eprime2)
      REAL*8 X, Y(5), YPRIME(5), NUI, eprime, eprime2
       REAL E, K, EPS, TI, EF, EFINF, NINF, DI, DE, VINF, C1, K1, A, B1, B2, B3, B4
        COMMON/CONST/E, K, EPS, TI, EF, EFINF, NINF, DI, DE, VIO, VINF, C1, K1, A
      VI = C1 * (Y(3) **K1)
      VIT = VI / VIO
      Following constants are the bracketed values in Equations 12-16.
C
      A is left as a variable.
C-
C
      B1 = ((E*EPS)/(K*TI)) * A
      B1 = 3.86E5 * A
C
      B2 = ((E*EFINF)/(K*TI)) * A
      B2 = 2.32E4 * A
C
      B3 = ((E*NINF) / (EF*EPS)) * A
      B3 = 9.04E5 * A
C
      B4 = ((VINF*K*TI)/(E*DE*EFINF)) * A
      B4 = 2.62E-21 * A
C
      Alpha = 2-body recombination coefficient (fm. Laser Kinetics
C
      Handbook (AFWL-TR-74-216, 1974)) (cm3/sec)
```

Alrha = 9.e-8

```
C-----
 C FIVE FIRST ORDER EQUATIONS - Equations 12-16
C--
С
     Ni
     YPRIME(1) = (B * Y(1) * Y(3)) - Y(5)
С
      YPRIME(2) = -(B * Y(2) * Y(3)) + Y(4)
С
      YPRIME(3) = B3 * (Y(1) - Y(2))
C
      je YPRIME(4) = -B4 * Y(2) * (VIT - (ALPHA * Y(1)))
C
      ji
      YPRIME(5) = B4 * Y(2) * (VIT - (ALPHA * Y(1)))
С
  -- Diagnostic Check of first, second derivatives-----
C-
C
      eprime = y(1) - y(2)
      eprime2 = yprime(1) - yprime(2)
С
      RETURN
      END
```

| C | IMSL ROUTIN  | E NAME | - DGEAR  | DGEA0010<br>DGEA0020 |  |
|---|--|--------|--|----------------------|--|
|   | -modified to return # of steps via variable "step" in subroutine cal |        |  |                      |  |
| C | COMPUTER   |        | - IBM/DOUBLE   | DGEA0040<br>DGEA0050 |  |
| C |  |        |  | DGEA0060             |  |
| C | LATEST REVI  | SION   | - NOVEMBER 1, 1984   | DGEA0070             |  |
| C |  |        |  | DGEA0080             |  |
| C | PURPOSE  |        | - DIFFERENTIAL EQUATION SOLVER - VARIABLE ORDER  |                      |  |
| C |  |        | ADAMS PREDICTOR CORRECTOR METHOD OR  | DGEA0100             |  |
| C |  |        | GEARS METHOD   | DGEA0110             |  |
| C | TTONOR   |        | - CALL DGEAR (N, FCN, FCNJ, X, H, Y, XEND, TOL, METH,                                  | DGEA0120<br>DGEA0130 |  |
| C | USAGE  |        | MITER, INDEX, IWK, WK, IER)  | DGEA0130             |  |
| C |  |        | MITER, INDEA, INK, NK, IER,  | DGEA0150             |  |
| C | ARGUMENTS  | N      | - INPUT NUMBER OF FIRST-ORDER DIFFERENTIAL   | DGEA0160             |  |
| C | .2.00.   | -      | EOUATIONS.   | DGEA0170             |  |
| C |  | FCN    | - NAME OF SUBROUTINE FOR EVALUATING FUNCTIONS.   | DGEA0180             |  |
| С |  |        | (INPUT)  | DGEA0190             |  |
| С |  |        | THE SUBROUTINE ITSELF MUST ALSO BE PROVIDED  | DGEA0200             |  |
| C |  |        | BY THE USER AND IT SHOULD BE OF THE  | DGEA0210             |  |
| C |  |        | FOLLOWING FORM   | DGEA0220             |  |
| C |  |        | SUBROUTINE FCN (N,X,Y,YPRIME)  | DGEA0230             |  |
| C |  |        | REAL X,Y(N),YPRIME(N)  | DGEA0240<br>DGEA0250 |  |
| C |  |        |  | DGEA0250             |  |
| C |  |        |  | DGEA0270             |  |
| C |  |        | FCN SHOULD EVALUATE YPRIME(1),,YPRIME(N)   |                      |  |
| C |  |        | GIVEN N, X, AND Y(1),, Y(N) . YPRIME(I)  | DGEA0290             |  |
| C |  |        | IS THE FIRST DERIVATIVE OF Y(I) WITH   | DGEA0300             |  |
| C |  |        | RESPECT TO X.  | DGEA0310             |  |
| C |  |        | FCN MUST APPEAR IN AN EXTERNAL STATEMENT IN  |                      |  |
| C |  |        | THE CALLING PROGRAM AND N,X,Y(1),,Y(N)   |                      |  |
| C |  | FCNJ   | MUST NOT BE ALTERED BY FCN NAME OF THE SUBROUTINE FOR COMPUTING THE                    | DGEA0340<br>DGEA0350 |  |
| C |  | FCNU   | JACOBIAN MATRIX OF PARTIAL DERIVATIVES.  | DGEA0350             |  |
| C |  |        | (INPUT)  | DGEA0370             |  |
| C |  |        | THE SUBROUTINE ITSELF MUST ALSO BE PROVIDED  |                      |  |
| C |  |        | BY THE USER.   | DGEA0390             |  |
| C |  |        | IF MITER=1 IT SHOULD BE OF THE FOLLOWING   | DGEA0400             |  |
| C |  |        | FORM   | DGEA0410             |  |
| C |  |        | SUBROUTINE FCNJ (N, X, Y, PD)  | DGEA0420             |  |
| C |  |        | REAL X,Y(N),PD(N,N)  | DGEA0430             |  |
| C |  |        | •  | DGEA0440<br>DGEA0450 |  |
| C |  |        | FCNJ MUST EVALUATE PD(I,J), THE PARTIAL  | DGEA0450             |  |
| C |  |        | DERIVATIVE OF YPRIME(I) WITH RESPECT TO  | DGEA0470             |  |
| C |  |        | Y(J), FOR I=1, N AND J=1, N.   | DGEA0480             |  |
| C |  |        | IF MITER= -1 IT SHOULD BE OF THE FOLLOWING   | DGEA0490             |  |
| C |  |        | FORM   | DGEA0500             |  |
| C |  |        | SUBROUTINE FCNJ (N,X,Y,PD)   | DGEA0510             |  |
| C |  |        | REAL X,Y(N),PD(1)  | DGEA0520             |  |
| C |  |        | ·  | DGEA0530             |  |
| C |  |        | FORT MICH EVALUATE DE IN BAND CHORACE MODE   | DGEA0540             |  |
| C |  |        | FCNJ MUST EVALUATE PD IN BAND STORAGE MODE.  THAT IS, PD(N*(J-I+NLC)+I) IS THE PARTIAL |                      |  |
| C |  |        |  | DGEA0570             |  |
| C |  |        | Y(J). NLC IS THE NUMBER OF LOWER   | DGEA0580             |  |
| C |  |        | CODIAGONALS FOR THE BAND MATRIX.   | DGEA0590             |  |
| C |  |        | FCNJ MUST APPEAR IN AN EXTERNAL STATEMENT I  |                      |  |
| C |  |        | THE CALLING PROGRAM AND N, X, Y(1),, Y(N)  | DGEA0610             |  |
|   |  |        |  |                      |  |

| C      |           |   | DGEA0620                         |
|--------|-----------|---|----------------------------------|
| C      |           | FCNJ IS USED ONLY IF MITER IS EQUAL TO 1 OR -1. OTHERWISE A DUMMY ROUTINE CAN | DGEA0630                         |
| C      |           | 1 OR -1. OTHERWISE A DUMMY ROUTINE CAN  | DGEA0640                         |
| C      |           | BE SUBSTITUTED. SEE REMARK 1.   | DGEA0650                         |
| C      | Х -       | INDEPENDENT VARIABLE. (INPUT AND OUTPUT)                                      | DGEA0650<br>DGEA0660<br>DGEA0670 |
| C      |           |   | DGEA0670                         |
| C      |           | AND IS USED ONLY ON THE FIRST CALL.   | DGEA0680                         |
| C      |           | ON OUTPUT, X IS REPLACED WITH THE CURRENT                                     |                                  |
| C      |           | VALUE OF THE INDEPENDENT VARIABLE AT WHICH                                    | HDGEA0700                        |
| C      |           | INTEGRATION HAS BEEN COMPLETED.   | DGEA0710                         |
| C      | H         | - INPUT/OUTPUT.   | DGEA0720                         |
| C      |           | ON INPUT, H CONTAINS THE NEXT STEP SIZE IN                                    |                                  |
| C      |           | X. H IS USED ONLY ON THE FIRST CALL.  | DGEA0740                         |
| C      |           | ON OUTPUT, H CONTAINS THE STEP SIZE USED LAST, WHETHER SUCCESSFULLY OR NOT.   | DGEA0750                         |
| C      |           | LAST, WHETHER SUCCESSFULLY OR NOT.  | DGEA0760                         |
| C      | Υ -       | DEPENDENT VARIABLES, VECTOR OF LENGTH N.                                      | DGEA0770                         |
| C      |           | (INPUT AND OUTPUT)  | DGEA0780<br>DGEA0790<br>DGEA0800 |
| C      |           | ON INPUT, Y(1),,Y(N) SUPPLY INITIAL   | DGEA0790                         |
| C      |           | VALUES.   | DGEA0800                         |
| C      |           | ON OUTPUT, Y(1),,Y(N) ARE REPLACED WITH                                       |                                  |
| C      |           |   | DGEA0820                         |
| C      | XEND -    | INPUT VALUE OF X AT WHICH SOLUTION IS DESIRED                                 |                                  |
| C      |           | NEXT. INTEGRATION WILL NORMALLY GO  |                                  |
| C      |           | BEYOND XEND AND THE ROUTINE WILL INTERPOLAT                                   |                                  |
| C      |           | TO $X = XEND$ .   | DGEA0860                         |
| C      |           |   | DGEA0870                         |
| C      |           | ZERO (X AND H AS SPECIFIED ON INPUT).   | DGEA0880                         |
| C      | TOL       | - INPUT RELATIVE ERROR BOUND. TOL MUST BE                                     |                                  |
| C      |           | GREATER THAN ZERO. TOL IS USED ONLY ON THE                                    |                                  |
| C      |           | FIRST CALL UNLESS INDEX IS EQUAL TO -1.                                       |                                  |
| C      |           |   | DGEA0920                         |
| C      |           | MAGNITUDE LARGER THAN THE UNIT ROUNDOFF                                       | DGEA0930                         |
| C      |           | BUT GENERALLY NOT LARGER THAN .001.   | DGEA0940                         |
| C      |           |   | DGEA0950                         |
| C      |           |   | DGEA0960                         |
| C      |           | ROOT-MEAN-SQUARE NORM (EUCLIDEAN NORM   | DGEA0970                         |
| C      |           |   | DGEA0980                         |
| C      |           | WEIGHTS IS COMPUTED INTERNALLY AND STORED                                     | DGEA0990                         |
| C      |           | IN WORK VECTOR WK. INITIALLY YMAX(I) IS                                       | DGEA1000                         |
| C      |           | THE ABSOLUTE VALUE OF Y(I), WITH A DEFAULT                                    |                                  |
| C      |           | VALUE OF ONE IF Y(I) IS EQUAL TO ZERO.  | DGEA1020                         |
| C      |           | THEREAFTER, YMAX(I) IS THE LARGEST VALUE                                      | DGEA1030                         |
| C      |           | OF THE ABSOLUTE VALUE OF Y(I) SEEN SO FAR,                                    | DGEA1040                         |
| C      |           | OR THE INITIAL VALUE OF YMAX(I) IF THAT IS                                    | DGEA1050                         |
| C      |           | LARGER.   | DGEA1060                         |
| C      | METH      | - INPUT BASIC METHOD INDICATOR.   | DGEA1070                         |
| C      |           | USED ONLY ON THE FIRST CALL UNLESS INDEX IS                                   |                                  |
| C<br>C |           | EQUAL TO -1.  | DGEA1090                         |
| C      |           | METH = 1, IMPLIES THAT THE ADAMS METHOD IS                                    | DGEA1100                         |
| C      |           | TO BE USED.   | DGEA1110                         |
| C      |           | METH = 2, IMPLIES THAT THE STIFF METHODS OF                                   | DGEA1120                         |
| C      |           | GEAR, OR THE BACKWARD DIFFERENTIATION   | DGEA1130                         |
| C<br>C | ) AT INTO | FORMULAE ARE TO BE USED.  | DGEA1140                         |
| C      | MITER     | - INPUT ITERATION METHOD INDICATOR.   | DGEA1150                         |
| C      |           | MITER = 0, IMPLIES THAT FUNCTIONAL  | DGEA1160                         |
| C      |           | ITERATION IS USED. NO PARTIAL   | DGEA1170                         |
| C      |           | DERIVATIVES ARE NEEDED. A DUMMY FCNJ  | DGEA1180                         |
| C      |           | CAN BE USED.  | DGEA1190                         |
| C      |           | MITER = 1, IMPLIES THAT THE CHORD METHOD                                      |                                  |
| C      |           | IS USED WITH AN ANALYTIC JACOBIAN. FOR  | DGEA1210                         |
| C .    |           | THIS METHOD, THE USER SUPPLIES  | DGEA1220                         |
| C .    |           | SUBROUTINE FCNJ.  | DGEA1230                         |

```
MITER = 2, IMPLIES THAT THE CHORD METHOD
                                                       DGEA1240
            IS USED WITH THE JACOBIAN CALCULATED
                                                        DGEA1250
             INTERNALLY BY FINITE DIFFERENCES.
                                                        DGEA1260
             A DUMMY FCNJ CAN BE USED.
                                                        DGEA1270
          MITER = 3, IMPLIES THAT THE CHORD METHOD DGEA1280
            IS USED WITH THE JACOBIAN REPLACED BY DGEA1290
             A DIAGONAL APPROXIMATION BASED ON A
                                                        DGEA1300
             DIRECTIONAL DERIVATIVE.
                                                        DGEA1310
             A DUMMY FCNJ CAN BE USED.
                                                        DGEA1320
          MITER = -1 OR -2, IMPLIES USE THE SAME DGEA1330
          METHOD AS FOR MITER= 1 OR 2, RESPECTIVELY, DGEA1340
            BUT USING A BANDED JACOBIAN MATRIX. IN DGEA1350
             THESE TWO CASES BANDWIDTH INFORMATION DGEA1360
                                                       DGEA1370
             MUST BE PASSED TO DGEAR THROUGH THE
             COMMON BLOCK
                                                        DGEA1380
                COMMON /DBAND/ NLC, NUC
                                                        DGEA1390
                   NUC=NUMBER OF LOWER CODIAGONALS DGEA1410
OUTPUT PARAMETER VICEO
             WHERE NLC=NUMBER OF LOWER CODIAGONALS
INDEX
      - INPUT AND OUTPUT PARAMETER USED TO INDICATE
                                                       DGEA1420
           THE TYPE OF CALL TO THE SUBROUTINE. ON
                                                        DGEA1430
           OUTPUT INDEX IS RESET TO 0 IF INTEGRATION
                                                       DGEA1440
           WAS SUCCESSFUL. OTHERWISE, THE VALUE OF
                                                        DGEA1450
           INDEX IS UNCHANGED.
                                                         DGEA1460
         ON INPUT, INDEX = 1, IMPLIES THAT THIS IS THE DGEA1470
           FIRST CALL FOR THIS PROBLEM.
                                           DGEA1480
        ON INPUT, INDEX = 0, IMPLIES THAT THIS IS NOT DGEA1490
          THE FIRST CALL FOR THIS PROBLEM. DGEA1500
       THE FIRST CALL FOR THIS PROBLEM. DGEA1500
ON INPUT, INDEX = -1, IMPLIES THAT THIS IS NOTDGEA1510
       THE FIRST CALL FOR THIS PROBLEM, AND THE DGEA1520
USER HAS RESET TOL. DGEA1530
ON INPUT, INDEX = 2, IMPLIES THAT THIS IS NOT DGEA1540
          THE FIRST CALL FOR THIS PROBLEM. INTEGRATIONDGEA1550
          IS TO CONTINUE AND XEND IS TO BE HIT EXACTLYDGEA1560
           (NO INTERPOLATION IS DONE). THIS VALUE OF DGEA1570
           INDEX ASSUMES THAT XEND IS BEYOND THE DGEA1580
            CURRENT VALUE OF X.
                                                        DGEA1590
       ON INPUT, INDEX = 3, IMPLIES THAT THIS IS NOT DGEA1600
           THE FIRST CALL FOR THIS PROBLEM. INTEGRATIONDGEA1610
           IS TO CONTINUE AND CONTROL IS TO BE RETURNEDDGEA1620
           TO THE CALLING PROGRAM AFTER ONE STEP. XEND DGEA1630
            IS IGNORED.
                                                         DGEA1640
IWK
         INTEGER WORK VECTOR OF LENGTH N. USED ONLY IF DGEA1650
            MITER = 1 OR 2
WK
       - REAL WORK VECTOR OF LENGTH 4*N+NMETH+NMITER.
           THE VALUE OF NMETH DEPENDS ON THE VALUE OF
              IF METH IS EQUAL TO 1,
                                                         DGEA1700
               NMETH IS EQUAL TO N*13.
                                                         DGEA1710
              IF METH IS EQUAL TO 2,
                                                         DGEA1720
               NMETH IS EQUAL TO N*6.
                                                         DGEA1730
           THE VALUE OF NMITER DEPENDS ON THE VALUE OF DGEA1740
              MITER.
                                                        DGEA1750
             NMITER IS EQUAL TO 1 OR 2,

IF MITER IS EQUAL TO -1 OR -2,

NMITER IS EQUAL TO -1 OR -2,
              IF MITER IS EQUAL TO 1 OR 2,
                                                         DGEA1760
                                                        DGEA1770
                                                        DGEA1780
              NMITER IS EQUAL TO (2*NLC+NUC+3)*N DGEA1790
              WHERE NLC=NUMBER OF LOWER CODIAGONALS DGEA1800
                      NUC=NUMBER OF UPPER CODIAGONALS DGEA1810
           IF MITER IS EQUAL TO 3,
                                                         DGEA1820
              NMITER IS EQUAL TO N.
                                                        DGEA1830
              IF MITER IS EQUAL TO 0,
                                                        DGEA1840
               NMITER IS EQUAL TO 1.
                                                        DGEA1850
```

```
WK MUST REMAIN UNCHANGED BETWEEN SUCCESSIVE DGEA1860
C
C
                            CALLS DURING INTEGRATION.
                                                                         DGEA1870
C
                        - ERROR PARAMETER. (OUTPUT)
                                                                         DGEA1880
C
                                                                         DGEA1890
                          WARNING ERROR
                            IER = 33, IMPLIES THAT X+H WILL EQUAL X ON DGEA1900
                              THE NEXT STEP. THIS CONDITION DOES NOT
C
                                                                       DGEA1910
C
                              FORCE THE ROUTINE TO HALT. HOWEVER, IT
                                                                        DGEA1920
C
                              DOES INDICATE ONE OF TWO CONDITIONS.
                                                                        DGEA1930
C
                              THE USER MIGHT BE REQUIRING TOO MUCH
                                                                        DGEA1940
C
                              ACCURACY VIA THE INPUT PARAMETER TOL.
                                                                        DGEA1950
C
                              IN THIS CASE THE USER SHOULD CONSIDER
                                                                        DGEA1960
C
                              INCREASING THE VALUE OF TOL. THE OTHER
                                                                        DGEA1970
C
                              CONDITION WHICH MIGHT GIVE RISE TO THIS
                                                                        DGEA1980
C
                              ERROR MESSAGE IS THAT THE SYSTEM OF
                                                                         DGEA1990
C
                                                                         DGEA2000
                              DIFFERENTIAL EQUATIONS BEING SOLVED
C
                              IS STIFF (EITHER IN GENERAL OR OVER
                                                                         DGEA2010
C
                              THE SUBINTERVAL OF THE PROBLEM BEING
                                                                         DGEA2020
                              SOLVED AT THE TIME OF THE ERROR). IN
C
                                                                         DGEA2030
C
                              THIS CASE THE USER SHOULD CONSIDER
                                                                         DGEA2040
C
                              USING A NONZERO VALUE FOR THE INPUT
                                                                         DGEA2050
C
                              PARAMETER MITER.
                                                                         DGEA2060
C
                          WARNING WITH FIX ERROR
                                                                         DGEA2070
                            IER = 66, IMPLIES THAT THE ERROR TEST
C
                                                                         DGEA2080
C
                              FAILED. H WAS REDUCED BY .1 ONE OR MORE
                                                                        DGEA2090
C
                              TIMES AND THE STEP WAS TRIED AGAIN
                                                                         DGEA2100
C
                              SUCCESSFULLY.
                                                                         DGEA2110
C
                            IER = 67, IMPLIES THAT CORRECTOR
                                                                         DGEA2120
C
                              CONVERGENCE COULD NOT BE ACHIEVED.
                                                                         DGEA2130
C
                              H WAS REDUCED BY .1 ONE OR MORE TIMES AND DGEA2140
C
                              THE STEP WAS TRIED AGAIN SUCCESSFULLY.
                                                                        DGEA2150
C
                          TERMINAL ERROR
                                                                          DGEA2160
C
                            IER = 132, IMPLIES THE INTEGRATION WAS
                                                                         DGEA2170
C
                              HALTED AFTER FAILING TO PASS THE ERROR
                                                                         DGEA2180
C
                              TEST EVEN AFTER REDUCING H BY A FACTOR
                                                                         DGEA2190
C
                              OF 1.0E10 FROM ITS INITIAL VALUE.
                                                                          DGEA2200
C
                               SEE REMARKS.
                                                                         DGEA2210
                            IER = 133, IMPLIES THE INTEGRATION WAS
C
                                                                         DGEA2220
                              HALTED AFTER FAILING TO ACHIEVE
                                                                         DGEA2230
C
                              CORRECTOR CONVERGENCE EVEN AFTER
                                                                          DGEA2240
C
                              REDUCING H BY A FACTOR OF 1.0E10 FROM
                                                                         DGEA2250
C
                              ITS INITIAL VALUE. SEE REMARKS.
                                                                          DGEA2260
                            IER = 134, IMPLIES THAT AFTER SOME INITIAL DGEA2270 SUCCESS, THE INTEGRATION WAS HALTED EITHERDGEA2280
C
C
C
                              BY REPEATED ERROR TEST FAILURES OR BY
                                                                          DGEA2290
C
                              A TEST ON TOL. SEE REMARKS.
                                                                          DGEA2300
                            IER = 135, IMPLIES THAT ONE OF THE INPUT
C
                                                                          DGEA2310
                              PARAMETERS N, X, H, XEND, TOL, METH, MITER, OR DGEA2320
C
                              INDEX WAS SPECIFIED INCORRECTLY.
                                                                          DGEA2330
C
                            IER = 136, IMPLIES THAT INDEX HAD A VALUE
                                                                          DGEA2340
C
                              OF -1 ON INPUT, BUT THE DESIRED CHANGES
                                                                          DGEA2350
C
                              OF PARAMETERS WERE NOT IMPLEMENTED
                                                                          DGEA2360
                              BECAUSE XEND WAS NOT BEYOND X.
                                                                          DGEA2370
C
                              INTERPOLATION TO X = XEND WAS PERFORMED.
                                                                         DGEA2380
                              TO TRY AGAIN, SIMPLY CALL AGAIN WITH
C
                                                                          DGEA2390
C
                              INDEX EQUAL TO -1 AND A NEW VALUE FOR
                                                                          DGEA2400
C
                               XEND.
                                                                          DGEA2410
C
                     Step -
                               # of integration steps taken
C
                                                                          DGEA2420
C
    PRECISION/HARDWARE
                        - SINGLE AND DOUBLE/H32
                                                                          DGEA2430
C
                         - SINGLE/H36,H48,H60
                                                                          DGEA2440
C
                                                                          DGEA2450
   REQD. IMSL ROUTINES - DGRCS, DGRIN, DGRPS, DGRST, LUDATF, LUELMF, LEQT1B, DGEA2460
```

|          |    |    | UERTST, UGETIO  | DGEA2470             |
|----------|----|----|---|----------------------|
|          |    |    |   | DGEA2480             |
| NOTATION |    |    | - INFORMATION ON SPECIAL NOTATION AND   | DGEA2490             |
|          |    |    |   | DGEA2500             |
|          |    |    | INTRODUCTION OR THROUGH IMSL ROUTINE UHELP  | DGEA2510             |
|          |    |    |   | DGEA2520             |
| REMAR    | KS | 1. | THE EXTERNAL SUBROUTINE FCNJ IS USED ONLY WHEN  | DGEA2530             |
|          |    |    | INPUT PARAMETER MITER IS EQUAL TO 1 OR -1. OTHERWISE,   | DGEA2540             |
|          |    |    |   | DGEA2550             |
|          |    |    |   | DGEA2560             |
|          |    |    |   | DGEA2570             |
|          |    |    | INTEGER N   | DGEA2580             |
|          |    |    | REAL Y(N), PD(N, N), X  | DGEA2590<br>DGEA2600 |
|          |    |    | RETURN<br>END   | DGEA2610             |
|          |    | 2  | AFTER THE INITIAL CALL, IF A NORMAL RETURN OCCURRED   | DGEA2620             |
|          |    | ۷. | (IER=0) AND A NORMAL CONTINUATION IS DESIRED, SIMPLY  | DGEA2630             |
|          |    |    | RESET XEND AND CALL DGEAR AGAIN. ALL OTHER  | DGEA2640             |
|          |    |    | PARAMETERS WILL BE READY FOR THE NEXT CALL. A CHANGE  | DGEA2650             |
|          |    |    | OF PARAMETERS WITH INDEX EQUAL TO -1 CAN BE MADE  | DGEA2660             |
|          |    |    | AFTER EITHER A SUCCESSFUL OR AN UNSUCCESSFUL RETURN.  | DGEA2670             |
|          |    | 3. |   | DGEA2680             |
|          |    |    | PRESERVED BETWEEN CALLS TO DGEAR. IF IT IS NECESSARY  | DGEA2690             |
|          |    |    | FOR THE COMMON BLOCKS TO EXIST IN THE CALLING PROGRAM   | DGEA2700             |
|          |    |    | THE FOLLOWING STATEMENTS SHOULD BE INCLUDED   | DGEA2710             |
|          |    |    | COMMON /DBAND/ NLC, NUC   | DGEA2720             |
|          |    |    | COMMON /GEAR/ DUMMY(48), SDUMMY(4), IDUMMY(38)  | DGEA2730             |
|          |    |    | WHERE DUMMY, SDUMMY, AND IDUMMY ARE VARIABLE NAMES NOT  |                      |
|          |    |    | USED ELSEWHERE IN THE CALLING PROGRAM. (FOR DOUBLE  | DGEA2750             |
|          |    |    | PRECISION DUMMY IS TYPE DOUBLE AND SDUMMY IS TYPE REAL)   |                      |
|          |    | 4. | THE CHOICE OF VALUES FOR METH AND MITER MAY REQUIRE   | DGEA2770             |
|          |    |    | SOME EXPERIMENTATION, AND ALSO SOME CONSIDERATION OF  | DGEA2780             |
|          |    |    | THE NATURE OF THE PROBLEM AND OF STORAGE REQUIREMENTS. THE PRIME CONSIDERATION IS STIFFNESS. IF | DGEA2790<br>DGEA2800 |
|          |    |    | THE PRIME CONSIDERATION IS STIFFNESS. IF THE PROBLEM IS NOT STIFF, THE BEST CHOICE IS PROBABLY  |                      |
|          |    |    | METH = 1 WITH MITER = 0. IF THE PROBLEM IS STIFF TO A   | DGEA2810             |
|          |    |    | SIGNIFICANT DEGREE, THEN METH SHOULD BE 2 AND MITER   | DGEA2830             |
|          |    |    | SHOULD BE 1,2,-1,-2 OR 3. IF THE USER HAS NO KNOWLEDGE  |                      |
|          |    |    | OF THE INHERENT TIME CONSTANTS OF THE PROBLEM, WITH   | DGEA2850             |
|          |    |    | WHICH TO PREDICT ITS STIFFNESS, ONE WAY TO DETERMINE  | DGEA2860             |
|          |    |    | THIS IS TO TRY METH = 1 AND MITER = 0 FIRST, AND LOOK   | DGEA2870             |
|          |    |    | AT THE BEHAVIOR OF THE SOLUTION COMPUTED AND THE STEP   | DGEA2880             |
|          |    |    | SIZES USED. IF THE TYPICAL VALUES OF H ARE MUCH   | DGEA2890             |
|          |    |    | SMALLER THAN THE SOLUTION BEHAVIOR WOULD SEEM TO  | DGEA2900             |
|          |    |    | REQUIRE (THAT IS, MORE THAN 100 STEPS ARE TAKEN OVER  | DGEA2910             |
|          |    |    | AN INTERVAL IN WHICH THE SOLUTIONS CHANGE BY LESS   | DGEA2920             |
|          |    |    | THAN ONE PERCENT), THEN THE PROBLEM IS PROBABLY STIFF   | DGEA2930             |
|          |    |    | AND THE DEGREE OF STIFFNESS CAN BE ESTIMATED FROM THE   | DGEA2940             |
|          |    |    | VALUES OF H USED AND THE SMOOTHNESS OF THE SOLUTION.  | DGEA2950             |
|          |    |    | IF THE DEGREE OF STIFFNESS IS ONLY SLIGHT, IT MAY BE  | DGEA2960             |
|          |    |    | THAT METH=1 IS MORE EFFICIENT THAN METH=2. EXPERIMENTATION WOULD BE REQUIRED TO DETERMINE THIS. | DGEA2970             |
|          |    |    | REGARDLESS OF METH, THE LEAST EFFECTIVE VALUE OF  | DGEA2980<br>DGEA2990 |
|          |    |    | MITER IS 0, AND THE MOST EFFECTIVE IS 1,-1,2,OR -2.   | DGEA2990             |
|          |    |    | MITER = 3 IS GENERALLY SOMEWHERE IN BETWEEN. SINCE  | DGEA3000             |
|          |    |    | THE STORAGE REQUIREMENTS GO UP IN THE SAME ORDER AS   | DGEA3010             |
|          |    |    | EFFECTIVENESS, TRADE-OFF CONSIDERATIONS ARE   | DGEA3030             |
|          |    |    | NECESSARY. FOR REASONS OF ACCURACY AND SPEED, THE   | DGEA3040             |
|          |    |    | CHOICE OF ABS (MITER) =1 IS GENERALLY PREFERRED TO  | DGEA3050             |
|          |    |    | ABS (MITER) = 2, UNLESS THE SYSTEM IS FAIRLY COMPLICATED  | DGEA3060             |
|          |    |    | (AND FCNJ IS THUS NOT FEASIBLE TO CODE). THE  | DGEA3070             |
|          |    |    | ACCURACY OF THE FCNJ CALCULATION CAN BE CHECKED BY  | DGEA3080             |
|          |    |    |   |                      |

a

| С   |   |     | COMPARISON OF THE JACOBIAN WITH THAT GENERATED WITH                                 | DGEA3090 |
|-----|---|-----|---|----------|
| C   |   |     |   | DGEA3100 |
| C   |   |     |   | DGEA3110 |
| C   |   |     | LIKELY TO BE NEARLY AS EFFECTIVE AS ABS (MITER) =1 OR 2,                            |          |
| C   |   |     |   | DGEA3130 |
| C   |   |     |   | DGEA3140 |
| C   |   |     |   | DGEA3150 |
| Č   |   |     |   | DGEA3160 |
| C   |   |     | ·   | DGEA3170 |
| Ċ   |   |     | ·   | DGEA3180 |
| Č   |   |     | · · · · · · · · · · · · · · · · · · ·   | DGEA3190 |
| C   |   | 5.  |   | DGEA3200 |
| C   |   |     |   | DGEA3210 |
| C   |   |     |   | DGEA3220 |
| Ċ   |   |     |   | DGEA3230 |
| Č   |   |     |   | DGEA3240 |
| C   |   |     | ·   | DGEA3250 |
| C   |   |     |   | DGEA3260 |
| Č   |   |     |   | DGEA3270 |
| Č   |   |     |   | DGEA3280 |
| C   |   |     |   | DGEA3290 |
| Č   |   |     | AND SUBSEQUENT RUNS ON THE SAME OR SIMILAR PROBLEM                                  | DGEA3300 |
| C   |   |     | SHOULD BE STARTED WITH AN APPROPRIATELY SMALLER                                     | DGEA3310 |
| C   |   |     | VALUE OF H.   | DGEA3320 |
| C   |   | 6.  |   | DGEA3330 |
| C   |   |     | , ,   | DGEA3340 |
| C   |   |     | COMMON BLOCK /GEAR/ ARE A. HUSED, THE STEP SIZE H LAST USED SUCCESSFULLY (DUMMY(8)) | DGEA3350 |
| Č   |   |     | (DUMMY (8))   | DGEA3360 |
| C   |   |     | B. NQUSED, THE ORDER LAST USED SUCCESSFULLY   | DGEA3370 |
| C   |   |     | (IDUMMY (6))  | DGEA3380 |
| C   |   |     | C. NSTEP, THE CUMULATIVE NUMBER OF STEPS TAKEN                                      | DGEA3390 |
| C   |   |     | (IDUMMY (7))  | DGEA3400 |
| Č   |   |     | D. NFE, THE CUMULATIVE NUMBER OF FCN EVALUATIONS                                    | DGEA3410 |
| Č   |   |     | /TDTMM72 / 0 \ \  | DGEA3420 |
| 0 0 |   |     | E. NJE, THE CUMULATIVE NUMBER OF JACOBIAN EVALUATIONS, AND HENCE ALSO OF MATRIX LU  | DGEA3430 |
| Č   |   |     | EVALUATIONS, AND HENCE ALSO OF MATRIX LU  | DGEA3440 |
| Č   |   |     | DECOMPOSITIONS (IDUMMY(9))  | DGEA3450 |
| C   |   | 7.  | THE NORMAL USAGE OF DGEAR MAY BE SUMMARIZED AS FOLLOWS                              |          |
| C   |   | , . | A. SET THE INITIAL VALUES IN Y.   | DGEA3470 |
| C   |   |     | B. SET N, X, H, TOL, METH, AND MITER.   | DGEA3480 |
| C   |   |     | C. SET XEND TO THE FIRST OUTPUT POINT, AND INDEX TO 1.                              |          |
| C   |   |     | D. CALL DGEAR   | DGEA3500 |
| C   |   |     | E. EXIT IF IER IS GREATER THAN 128.   | DGEA3510 |
| Č   |   |     | F. OTHERWISE, DO DESIRED OUTPUT OF Y.   | DGEA3520 |
| C   |   |     | G. EXIT IF THE PROBLEM IS FINISHED.   | DGEA3530 |
| C   |   |     | H. OTHERWISE, RESET XEND TO THE NEXT OUTPUT POINT, AND                              |          |
| Č   |   |     | RETURN TO STEP D.   | DGEA3550 |
| C   |   | 8.  | THE ERROR WHICH IS CONTROLLED BY WAY OF THE PARAMETER                               | DGEA3560 |
| Ċ   |   |     | TOL IS AN ESTIMATE OF THE LOCAL TRUNCATION ERROR, THAT                              |          |
| C   |   |     | IS, THE ERROR COMMITTED ON TAKING A SINGLE STEP WITH                                |          |
| C   |   |     | THE METHOD, STARTING WITH DATA REGARDED AS EXACT. THIS                              |          |
| Č   |   |     | IS TO BE DISTINGUISHED FROM THE GLOBAL TRUNCATION                                   | DGEA3600 |
| Č   |   |     | ERROR, WHICH IS THE ERROR IN ANY GIVEN COMPUTED VALUE                               |          |
| Č   |   |     | OF Y(X) AS A RESULT OF THE LOCAL TRUNCATION ERRORS                                  | DGEA3620 |
| Č   |   |     | FROM ALL STEPS TAKEN TO OBTAIN Y(X). THE LATTER ERROR                               |          |
| C   |   |     | ACCUMULATES IN A NON-TRIVIAL WAY FROM THE LOCAL                                     | DGEA3640 |
| Ċ   |   |     | ERRORS, AND IS NEITHER ESTIMATED NOR CONTROLLED BY                                  | DGEA3650 |
| C   |   |     | THE ROUTINE. SINCE IT IS USUALLY THE GLOBAL ERROR THAT                              |          |
| Č   |   |     | A USER WANTS TO HAVE UNDER CONTROL, SOME  | DGEA3670 |
| Ċ   |   |     | EXPERIMENTATION MAY BE NECESSARY TO GET THE RIGHT                                   | DGEA3680 |
| Č   |   |     |   | DGEA3690 |
| Č   | • |     | PROBLEM IS MATHEMATICALLY STABLE, AND THE METHOD USED                               |          |
|     |   |     |   |          |

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IS APPROPRIATELY STABLE, THEN THE GLOBAL ERROR AT A
                                                                           DGEA3710
                GIVEN X SHOULD VARY SMOOTHLY WITH TOL IN A MONOTONE
                                                                           DGEA3720
                 INCREASING MANNER.
                                                                           DGEA3730
                IF THE ROUTINE RETURNS WITH IER VALUES OF 132, 133,
                                                                           TGEA3740
                OR 134, THE USER SHOULD CHECK TO SEE IF TOO MUCH
                                                                           DGEA3750
                ACCURACY IS BEING REQUIRED. THE USER MAY WISH TO
                                                                           DGEA3760
                SET TOL TO A LARGER VALUE AND CONTINUE. ANOTHER
                                                                           DGEA3770
                POSSIBLE CAUSE OF THESE ERROR CONDITIONS IS AN
                                                                           DGEA3780
                ERROR IN THE CODING OF THE EXTERNAL FUNCTIONS FCN
                                                                           DGEA3790
                OR FCNJ. IF NO ERRORS ARE FOUND, IT MAY BE NECESSARY
                                                                           DGEA3800
                TO MONITOR INTERMEDIATE QUANTITIES GENERATED BY THE
                                                                           DGEA3810
                ROUTINE. THESE QUANTITIES ARE STORED IN THE WORK VECTORDGEA3820
                WK AND INDEXED BY SPECIFIC ELEMENTS IN THE COMMON BLOCKDGEA3830
                 /GEAR/. IF IER IS 132 OR 134, THE COMPONENTS CAUSING
                                                                           DGEA3840
                THE ERROR TEST FAILURE CAN BE IDENTIFIED FROM LARGE
                                                                           DGEA3850
                 VALUES OF THE QUANTITY
                                                                           DGEA3860
                   WK(IDUMMY(11)+I)/WK(I), FOR I=1,...,N.
                                                                           DGEA3870
                ONE CAUSE OF THIS MAY BE A VERY SMALL BUT NONZERO
                                                                           DGEA3880
                 INITIAL VALUE OF ABS(Y(I)).
                                                                           DGEA3890
                 IF IER IS 133, SEVERAL POSSIBILITIES EXIST.
                                                                           DGEA3900
                IT MAY BE INSTRUCTIVE TO TRY DIFFERENT VALUES OF MITER.DGEA3910
                ALTERNATIVELY, THE USER MIGHT MONITOR SUCCESSIVE
                                                                           DGEA3920
                CORRECTOR ITERATES CONTAINED IN WK(IDUMMY(12)+I), FOR DGEA3930
                I=1,..., N. ANOTHER POSSIBILITY MIGHT BE TO MONITOR
                                                                           DGEA3940
                 THE JACOBIAN MATRIX, IF ONE IS USED, STORED, BY
                                                                           DGEA3950
                COLUMN, IN WK(IDUMMY(10)+I), FOR I=1,...,N*N IF ABS(MITER) IS EQUAL TO 1 OR 2, OR FOR I=1,...,N IF
                                                                           DGEA3960
                                                                           DGEA3970
                 MITER IS EQUAL TO 3.
                                                                           DGEA3980
                                                                           DGEA3990
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                                                                           DGEA4000
                                                                           DGEA4010
                        - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN DGEA4020
   WARRANTY
                            APPLIED TO THIS CODE. NO OTHER WARRANTY.
                                                                           DGEA4030
                            EXPRESSED OR IMPLIED, IS APPLICABLE.
                                                                           DGEA4040
                                                                           DGEA4050
C.
                                                                           -DGEA4060
                                                                           DGEA4070
      SUBROUTINE DGEAR (N, FCN, FCNJ, X, H, Y, XEND, TOL, METH, MITER, INDEX,
                                                                           DGEA4080
     1
                           IWK, WK, IER, step)
                                                                             +
                                    SPECIFICATIONS FOR ARGUMENTS
                                                                           DGEA4100
      INTEGER
                          N, METH, MITER, INDEX, IWK(1), IER, step
                                                                             +
      DOUBLE PRECISION
                          X,H,Y(N),XEND,TOL,WK(1)
                                                                           DGEA4120
                                    SPECIFICATIONS FOR LOCAL VARIABLES
                                                                           DGEA4130
                         NERROR, NSAVE1, NSAVE2, NPW, NY, NC, MFC, KFLAG,
                                                                           DGEA4140
      INTEGER
                         JSTART, NSQ, NQUSED, NSTEP, NFE, NJE, I, NO, NHCUT, KGO, DGEA4150
     1
     2
                         JER, KER, NN, NEQUIL, IDUMMY (21), NLC, NUC
                                                                            DGEA4160
      REAL
                          SDUMMY (4)
                                                                            DGEA4170
      DOUBLE PRECISION
                         T, HH, HMIN, HMAX, EPSC, UROUND, EPSJ, HUSED, TOUTP,
                                                                            DGEA4180
                         AYI, D, DN, SEPS, DUMMY (39)
                                                                            DGEA4190
      EXTERNAL
                          FCN, FCNJ
                                                                            DGEA4200
      COMMON / DBAND /
                          NLC, NUC
                                                                            DGEA4210
      COMMON /GEAR/
                         T, HH, HMIN, HMAX, EPSC, UROUND, EPSJ, HUSED, DUMMY,
                                                                            DGEA4220
                         TOUTP, SDUMMY, NC, MFC, KFLAG, JSTART, NSQ, NQUSED,
                                                                            DGEA4230
     1
     2
                         NSTEP, NFE, NJE, NPW, NERROR, NSAVE1, NSAVE2, NEQUIL, DGEA4240
     3
                          NY, IDUMMY, NO, NHCUT
                                                                            DGEA4250
                          SEPS/Z3410000000000000/
                                                                            DGEA4260
      DATA
C
                                    FIRST EXECUTABLE STATEMENT
                                                                            DGEA4270
      IF (MITER.GE.0) NLC = -1
                                                                            DGEA4280
      KER = 0
                                                                            DGEA4290
      JER = 0
                                                                            DGEA4300
      URCUND = SEPS
                                                                            DGEA4310
C
                                    COMPUTE WORK VECTOR INDICIES
                                                                            DGEA4320
```

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NERROR = N
                                                                         DGEA4330
      NSAVE1 = NERROR+N
                                                                         DGEA4340
      NSAVE2 = NSAVE1+N
                                                                         DGEA4350
      NY = NSAVE2+N
                                                                         DGEA4360
      IF (METH.EQ.1) NEQUIL = NY+13*N
                                                                         DGEA4370
      IF (METH.EQ.2) NEQUIL = NY+6*N
                                                                         DGEA4380
      NPW = NEQUIL + N
                                                                         DGEA4390
      IF (MITER.EO.O.OR.MITER.EO.3) NPW = NEOUIL
                                                                         DGEA4400
      MFC = 10*METH+IABS(MITER)
                                                                         DGEA4410
C
                                   CHECK FOR INCORRECT INPUT PARAMETERS DGEA4420
C
                                                                         DGEA4430
      IF (MITER.LT.-2.OR.MITER.GT.3) GO TO 85
                                                                         DGEA4440
      IF (METH.NE.1.AND.METH.NE.2) GO TO 85
                                                                         DGEA4450
      IF (TOL.LE.O.DO) GO TO 85
                                                                         DGEA4460
      IF (N.LE.0) GO TO 85
                                                                         DGEA4470
      IF ((X-XEND)*H.GE.O.DO) GO TO 85
                                                                         DGEA4480
      IF (INDEX.EQ.0) GO TO 10
                                                                         DGEA4490
      IF (INDEX.EQ.2) GO TO 15
                                                                          DGEA4500
      IF (INDEX.EQ.-1) GO TO 20
                                                                          DGEA4510
      IF (INDEX.EQ.3) GO TO 25
                                                                          DGEA4520
      IF (INDEX.NE.1) GO TO 85
                                                                          DGEA4530
C
                                   IF INITIAL VALUES OF YMAX OTHER THAN DGEA4540
C
                                     THOSE SET BELOW ARE DESIRED, THEY
                                                                          DGEA4550
0000
                                     SHOULD BE SET HERE. ALL YMAX(I)
                                                                          DGEA4560
                                     MUST BE POSITIVE. IF VALUES FOR
                                                                          DGEA4570
                                     HMIN OR HMAX, THE BOUNDS ON
                                                                          DGEA4580
                                     DABS (HH), OTHER THAN THOSE BELOW
                                                                          DGEA4590
C
                                     ARE DESIRED, THEY SHOULD BE SET
                                                                          DGEA4600
C
                                     BELOW.
                                                                          DGEA4610
      DO 5 I=1, N
                                                                          DGEA4620
         WK(I) = DABS(Y(I))
                                                                          DGEA4630
         IF (WK(I).EQ.0.D0) WK(I) = 1.D0
                                                                          DGEA4640
         WK(NY+I) = Y(I)
                                                                          DGEA4650
    5 CONTINUE
                                                                          DGEA4660
      NC = N
                                                                          DGEA4670
      T = X
                                                                          DGEA4680
      HH = H
                                                                          DGEA4690
      IF ((T+HH).EQ.T) KER = 33
                                                                          DGEA4700
      HMIN = DABS(H)
                                                                          DGEA4710
      HMAX = DABS(X-XEND)*10.D0
                                                                          DGEA4720
      EPSC = TOL
                                                                          DGEA4730
      JSTART = 0
                                                                          DGEA4740
      N0 = N
                                                                          DGEA4750
      NSQ = N0*N0
                                                                          DGEA4760
      EPSJ = DSQRT (UROUND)
                                                                          DGEA4770
      NHCUT = 0
                                                                          DGEA4780
      DUMMY(2) = 1.0D0
                                                                          DGEA4790
      DUMMY(14) = 1.0D0
                                                                          DGEA4800
      GO TO 30
                                                                          DGEA4810
C
                                   TOUTP IS THE PREVIOUS VALUE OF XEND
                                                                          DGEA4820
                                      FOR USE IN HMAX.
                                                                          DGEA4830
   10 HMAX = DABS (XEND-TOUTP) *10.D0
                                                                          DGEA4840
      GO TO 45
                                                                          DGEA4850
C
                                                                          DGEA4860
   15 HMAX = DABS (XEND-TOUTP) *10.D0
                                                                          DGEA4870
      IF ((T-XEND) *HH.GE.O.DO) GO TO 95
                                                                          DGEA4880
      GO TO 50
                                                                          DGEA4890
C
                                                                          DGEA4900
   20 IF ((T-XEND)*HH.GE.O.DO) GO TO 90
                                                                          DGEA4910
      JSTART = -1
                                                                          DGEA4920
      NC = N
                                                                          DGEA4930
      EPSC = TOL
                                                                          DGEA4940
```

```
DGEA4950
C
   25 IF ((T+HH).EQ.T) KER = 33
                                                                          DGEA4960
      write(*,*), 'error code = ', ker
                                                                          DGEA4970
   30 \text{ NN} = \text{NO}
                                                                           DGEA4980
      step = step + 1
                                                                            +
      write(*,*)'step = ',step
      CALL DGRST (FCN, FCNJ, WK (NY+1), WK, WK (NERROR+1), WK (NSAVE1+1),
                                                                          DGEA4990
     1 WK (NSAVE2+1), WK (NPW+1), WK (NEOUIL+1), IWK, NN, step)
                                                                          DGEA5010
C
      KGO = 1 - KFLAG
                                                                           DGEA5020
      GO TO (35,55,70,80), KGO
                                                                           DGEA5030
C
                                    KFLAG = 0, -1, -2, -3
                                                                           DGEA5040
   35 CONTINUE
                                                                           DGEA5050
                                   NORMAL RETURN FROM INTEGRATOR. THE
                                                                           DGEA5060
C
C
                                     WEIGHTS YMAX(I) ARE UPDATED. IF
                                                                           DGEA5070
000000000
                                     DIFFERENT VALUES ARE DESIRED, THEY DGEA5080
                                     SHOULD BE SET HERE. A TEST IS MADE DGEA5090
                                      FOR TOL BEING TOO SMALL FOR THE
                                                                           DGEA5100
                                     MACHINE PRECISION. ANY OTHER TESTS DGEA5110
                                     OR CALCULATIONS THAT ARE REQUIRED
                                                                          DGEA5120
                                      AFTER EVERY STEP SHOULD BE
                                                                           DGEA5130
                                      INSERTED HERE. IF INDEX = 3, Y IS
                                                                           DGEA5140
                                      SET TO THE CURRENT SOLUTION ON
                                                                           DGEA5150
                                      RETURN. IF INDEX = 2, HH IS
                                                                           DGEA5160
CC
                                      CONTROLLED TO HIT XEND (WITHIN
                                                                           DGEA5170
                                      ROUNDOFF ERROR), AND THEN THE
                                                                           DGEA5180
                                      CURRENT SOLUTION IS PUT IN Y ON
C
                                                                           DGEA5190
C
                                      RETURN. FOR ANY OTHER VALUE OF
                                                                           DGEA5200
C
                                      INDEX, CONTROL RETURNS TO THE
                                                                           DGEA5210
C
                                      INTEGRATOR UNLESS XEND HAS BEEN
                                                                           DGEA5220
C
                                     REACHED. THEN INTERPOLATED VALUES
                                                                           DGEA5230
C
                                     OF THE SOLUTION ARE COMPUTED AND
                                                                           DGEA5240
C
                                                                           DGEA5250
                                      STORED IN Y ON RETURN.
C
                                                                           DGEA5260
                                      IF INTERPOLATION IS NOT
C
                                     DESIRED, THE CALL TO DGRIN SHOULD
                                                                           DGEA5270
C
                                     BE REMOVED AND CONTROL TRANSFERRED DGEA5280
C
                                      TO STATEMENT 95 INSTEAD OF 105.
                                                                           DGEA5290
      D = 0.D0
                                                                           DGEA5300
      DO 40 I=1, N
                                                                           DGEA5310
         AYI = DABS(WK(NY+I))
                                                                           DGEA5320
         WK(I) = DMAX1(WK(I),AYI)
                                                                           DGEA5330
   40 D = D + (AYI/WK(I)) **2
                                                                           DGEA5340
      D = D*(UROUND/TOL)**2
                                                                           DGEA5350
      DN = N
                                                                           DGEA5360
      IF (D.GT.DN) GO TO 75
                                                                           DGEA5370
      IF (INDEX.EQ.3) GO TO 95
                                                                           DGEA5380
      IF (INDEX.EQ.2) GO TO 50
                                                                           DGEA5390
   45 IF ((T-XEND) *HH.LT.0.D0) GO TO 25
                                                                           DGEA5400
      NN = N0
                                                                           DGEA5410
      CALL DGRIN (XEND, WK(NY+1), NN, Y)
                                                                           DGEA5420
      X = XEND
                                                                           DGEA5430
      GO TO 105
                                                                           DGEA5440
   50 IF (((T+HH)-XEND)*HH.LE.O.DO) GO TO 25
                                                                           DGEA5450
      IF (DABS(T-XEND).LE.UROUND*DMAX1(10.D0*DABS(T),HMAX)) GO TO 95
                                                                           DGEA5460
      IF ((T-XEND) *HH.GE.O.DO) GO TO 95
                                                                           DGEA5470
      HH = (XEND-T) * (1.D0-4.D0*UROUND)
                                                                           DGEA5480
      JSTART = -1
                                                                           DGEA5490
      GO TO 25
                                                                           DGEA5500
C
                                    ON AN ERROR RETURN FROM INTEGRATOR,
                                                                           DGEA5510
C
                                      AN IMMEDIATE RETURN OCCURS IF
                                                                           DGEA5520
                                      KFLAG = -2, AND RECOVERY ATTEMPTS
                                                                          DGEA5530
```

```
C
                                       ARE MADE OTHERWISE. TO RECOVER, HH DGEA5540
 C
                                       AND HMIN ARE REDUCED BY A FACTOR
 C
                                                                             DGEA5550
                                       OF .1 UP TO 10 TIMES BEFORE GIVING DGEA5560
                                        UP.
    55 \text{ JER} = 66
                                                                             DGEA5570
    60 IF (NHCUT.EQ.10) GO TO 65
                                                                             DGEA5580
       NHCUT = NHCUT+1
                                                                             DGEA5590
       HMIN = HMIN*.1D0
                                                                             DGEA5600
       HH = HH*.1D0
                                                                             DGEA5610
       JSTART = -1
                                                                             DGEA5620
       GO TO 25
                                                                             DGEA5630
C
                                                                             DGEA5640
    65 IF (JER.EQ.66) JER = 132
                                                                             DGEA5650
       IF (JER.EQ.67) JER = 133
                                                                             DGEA5660
       GO TO 95
                                                                             DGEA5670
C
                                                                             DGEA5680
    70 JER = 134
                                                                             DGEA5690
       GO TO 95
                                                                             DGEA5700
C
                                                                             DGEA5710
   75 \text{ JER} = 134
                                                                             DGEA5720
      KFLAG = -2
                                                                            DGEA5730
      GO TO 95
                                                                            DGEA5740
C
                                                                            DGEA5750
   80 JER = 67
                                                                            DGEA5760
      GO TO 60
                                                                            DGEA5770
C
                                                                            DGEA5780
   85 JER = 135
                                                                            DGEA5790
      GO TO 110
                                                                            DGEA5800
C
                                                                            DGEA5810
   90 \text{ JER} = 136
                                                                            DGEA5820
      NN = N0
                                                                            DGEA5830
                                                                            DGEA5840
      CALL DGRIN (XEND, WK(NY+1), NN, Y)
      X = XEND
                                                                            DGEA5850
      GO TO 110
                                                                            DGEA5860
C
                                                                            DGEA5870
   95 X = T
                                                                            DGEA5880
      DO 100 I=1,N
                                                                            DGEA5890
  100 Y(I) = WK(NY+I)
                                                                            DGEA5900
 105 IF (JER.LT.128) INDEX = KFLAG
                                                                            DGEA5910
      TOUTP = X
                                                                            DGEA5920
      IF (KFLAG.EQ.0) H = HUSED
                                                                            DGEA5930
      IF (KFLAG.NE.O) H = HH
                                                                            DGEA5940
 110 IER = MAXO(KER, JER)
                                                                            DGEA5950
9000 CONTINUE
                                                                           DGEA5960
      IF (KER.NE.O.AND.JER.LT.128) CALL UERTST (KER,6HDGEAR )
                                                                           DGEA5970
      IF (JER.NE.0) CALL UERTST (JER,6HDGEAR )
                                                                           DGEA5980
9005 RETURN
                                                                           DGEA5990
     END
                                                                           DGEA6000
                                                                           DGEA6010
```

| C | IMSL ROUTINE NAME    | - DGRST  | DGRS0010<br>DGRS0020 |
|---|----------------------|--|----------------------|
|   | odified to print she | eath and diagnostic output to files "sheatha.dat   |                      |
|   | nd "diag.dat"        |  | +                    |
| C | COMPUTER             | - IBM/DOUBLE   | DGRS0050             |
| C |                      |  | DGRS0060             |
| C | LATEST REVISION      | - JUNE 1, 1982   | DGRS0070             |
| С |                      |  | DGRS0080             |
| С | PURPOSE              | - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR   | DGRS0090             |
| С |                      |  | DGRS0100             |
| C | PRECISION/HARDWARE   | - SINGLE AND DOUBLE/H32  | DGRS0110             |
| C |                      | - SINGLE/H36, H48, H60   | DGRS0120             |
| С |                      |  | DGRS0130             |
| C | REQD. IMSL ROUTINES  | - DGRCS, DGRPS, LUDATF, LUELMF, LEQT1B, UERTST,  | DGRS0140             |
| C |                      | UGETIO   | DGRS0150             |
| С |                      |  | DGRS0160             |
| С | NOTATION             | - INFORMATION ON SPECIAL NOTATION AND  | DGRS0170             |
| C |                      | CONVENTIONS IS AVAILABLE IN THE MANUAL   | DGRS0180             |
| C |                      | INTRODUCTION OR THROUGH IMSL ROUTINE UHELP   | DGRS0190             |
| C |                      | 1000 DV TVOT TVO DT DTGVING DECEDIND   | DGRS0200             |
| C | COPYRIGHT            | - 1982 BY IMSL, INC. ALL RIGHTS RESERVED.  | DGRS0210             |
| C | 1.73 C C A \$111137  | THE WARDANDS ONLY THAT THE TESTING HAS DEEN  | DGRS0220             |
| C | WARRANTY             | - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN APPLIED TO THIS CODE. NO OTHER WARRANTY, | DGRS0230             |
| C |                      | EXPRESSED OR IMPLIED, IS APPLICABLE.   | DGRS0250             |
| C |                      | EAFRESSED OR IMPLIED, IS APPLICABLE.   | DGRS0250             |
| C |                      |  | -DGRS0270            |
| C |                      |  | DGRS0280             |
|   | SUBROUTINE DGRST     | (FCN, FCNJ, Y, YMAX, ERROR, SAVE1, SAVE2, PW, EQUIL,                                     | DGRS0290             |
|   | 1                    | IPIV,NO,step)  | +                    |
| С | _                    | SPECIFICATIONS FOR ARGUMENTS   | DGRS0310             |
|   | INTEGER              | IPIV(1), NO  | DGRS0320             |
|   | DOUBLE PRECISION     | Y(NO,1), YMAX(1), ERROR(1), SAVE1(1), SAVE2(1),  | DGRS0330             |
|   | 1                    | PW(1), EQUIL(1), eprime, eprime(2)   | +                    |
| C |                      | SPECIFICATIONS FOR LOCAL VARIABLES   | DGRS0350             |
|   | INTEGER              | N, MF, KFLAG, JSTART, NQUSED, NSTEP, NFE, NJE, NSQ,                                      | DGRS0360             |
|   | 1                    | I, METH, MITER, NQ, L, IDOUB, MFOLD, NOLD, IRET, MEO,                                    | DGRS0370             |
|   | 2                    | MIO, IWEVAL, MAXDER, LMAX, IREDO, J, NSTEPJ, J1, J2,                                     | DGRS0380             |
|   | 3                    | M, IER, NEWQ, NPW, NERROR, NSAVE1, NSAVE2, NEQUIL, NY,                                   | DGRS0390             |
|   | 4                    | MITER1, IDUMMY(2), NLC, NUC, NWK, JER  | DGRS0400             |
|   | REAL                 | TQ(4)  | DGRS0410             |
|   | DOUBLE PRECISION     | T, H, HMIN, HMAX, EPS, UROUND, HUSED, EL(13), OLDLO,                                     | DGRS0420             |
|   | 1                    | TOLD, RMAX, RC, CRATE, EPSOLD, HOLD, FN, EDN, E, EUP,                                    | DGRS0430             |
|   | 2                    | BND, RH, R1, CON, R, HLO, RO, D, PHLO, PR3, D1, ENQ3, ENQ2                               | ·                    |
|   | 3<br>EXTERNAL        | PR2,PR1,ENQ1,EPSJ,DUMMY,tcum<br>FCN,FCNJ   | +<br>DGRS0460        |
|   | COMMON /DBAND/       | NLC, NUC   | DGRS0470             |
|   | COMMON / GEAR/       | T, H, HMIN, HMAX, EPS, UROUND, EPSJ, HUSED,  | DGRS0470             |
|   | 1                    | EL, OLDLO, TOLD, RMAX, RC, CRATE, EPSOLD, HOLD, FN,                                      | DGRS0480             |
|   | 2                    | EDN, E, EUP, BND, RH, R1, R, HL0, R0, D, PHL0, PR3, D1,                                  | DGRS0500             |
|   | 3                    | ENQ3, ENQ2, PR2, PR1, ENQ1, DUMMY, TQ,   | DGRS0510             |
|   | 4                    | N,MF,KFLAG,JSTART,NSQ,NQUSED,NSTEP,NFE,NJE,  | DGRS0510             |
|   | 5                    | NPW, NERROR, NSAVE1, NSAVE2, NEQUIL, NY,   | DGRS0520             |
|   | 6                    | I, METH, MITER, NQ, L, IDOUB, MFOLD, NOLD, IRET, MEO,                                    | DGRS0540             |
|   | 7                    | MIO, IWEVAL, MAXDER, LMAX, IREDO, J, NSTEPJ, J1, J2,                                     | DGRS0550             |
|   | 8                    | M, NEWQ, IDUMMY  | DGRS0560             |
| С |                      | FIRST EXECUTABLE STATEMENT   | DGRS0570             |
|   | open(unit=8,file     | ='sheatha.dat',status='unknown')   | +                    |
|   |                      | ='diag.dat', status='unknown')   | +                    |
|   | KFLAG = 0            |  | DGRS0580             |
|   | $TO_{i}D = T$        |  | DGRS0590             |
| C |                      | THIS ROUTINE PERFORMS ONE STEP OF  | DGRS0600             |
|   |                      |  |                      |

|                 | THE INTEGRATION OF A VALUE PROBLEM FOR A ORDINARY DIFFERENTIA  IF (JSTART.GT.0) GO TO 50  IF (JSTART.NE.0) GO TO 10  ON THE FIRST CALL, THE TO 1 AND THE INITIAL CALCULATED. RMAX IS RATIO BY WHICH H CAM IN A SINGLE STEP. IT 1.E4 TO COMPENSATE I INITIAL H, BUT THEN EQUAL TO 10. IF A FA (IN CORRECTOR CONVEL TEST), RMAX IS SET A NEXT INCREASE.  | SYSTEM OF DAL EQUATIONS. DE LE ORDER IS SET DE LE YDOT IS DE LE YDOT IS DE LE YDOT IS DE LE YDOT IS INCREASED DE LE YDOT IS INITIALLY DE LE YDOT THE SMALL DE LE YDOT THE SMALL DE LE YDOT THE SMALL DE LE YDOT THE Y | OGRS0610<br>OGRS0620<br>OGRS0630<br>OGRS0640<br>OGRS0650<br>OGRS0660<br>OGRS0660<br>OGRS0690<br>OGRS0710<br>OGRS0710<br>OGRS0720<br>OGRS0730<br>OGRS0740<br>OGRS0750 |
|-----------------|--|--|--|
|                 | CALL FCN (N,T,Y,SAVE1,eprime,eprime2) DO 5 I=1,N  5 Y(I,2) = H*SAVE1(I) METH = MF/10 MITER = MF-10*METH NQ = 1 L = 2 IDOUB = 3 RMAX = 1.D4 RC = 0.D0 CRATE = 1.D0 HOLD = H MFOLD = MF NSTEP = 0 NSTEPJ = 0 NFE = 1 NJE = 0 IRET = 3  |  | + DGRS0780 DGRS0800 DGRS0810 DGRS0820 DGRS0830 DGRS0840 DGRS0850 DGRS0860 DGRS0880 DGRS0890 DGRS0990 DGRS0910 DGRS0930 DGRS0940                                      |
| 000000000000000 | IF THE CALLER HAS CHA DGRCS IS CALLED TO COEFFICIENTS OF THE CALLER HAS CHANGED METH, THE CONSTANTS AND BND MUST BE RES COMPARISON FOR ERRO CURRENT ORDER NQ. E FOR INCREASING THE DECREASING THE ORDE TO TEST FOR CONVERG CORRECTOR ITERATES. HAS CHANGED H, Y MU IF H OR METH HAS BE IDOUB IS RESET TO L FURTHER CHANGES IN STEPS.  10 IF (MF.EQ.MFOLD) GO TO 25 MEO = METH MIO = MITER METH = MF/10 MITER = MF-10*METH MFOLD = MF IF (MITER.NE.MIO) IWEVAL = MITER IF (METH.EQ.MEO) GO TO 25 IDOUB = L+1 IRET = 1 | NGED METH, SET THE METHOD. IF THE I N, EPS, OR E, EDN, EUP, ET. E IS A RS OF THE UP IS TO TEST ORDER, EDN FOR R. BND IS USED ENCE OF THE IF THE CALLER ST BE RESCALED. EN CHANGED, + 1 TO PREVENT H FOR THAT MANY  | DGRS0990<br>DGRS1000<br>DGRS1010<br>DGRS1020<br>DGRS1030<br>DGRS1040<br>DGRS1050<br>DGRS1060<br>DGRS1070<br>DGRS1080<br>DGRS1090<br>DGRS1090                         |

```
15 CALL DGRCS (METH, NQ, EL, TQ, MAXDER)
                                                                       DGRS1230
                                                                       DGRS1240
   LMAX = MAXDER+1
   RC = RC*EL(1)/OLDL0
                                                                       DGRS1250
   OLDLO = EL(1)
                                                                       DGRS1260
20 \text{ FN} = \text{N}
                                                                       DGRS1270
  EDN = FN*(TQ(1)*EPS)**2
                                                                       DGRS1280
   E = FN*(TQ(2)*EPS)**2
                                                                       DGRS1290
   EUP = FN*(TO(3)*EPS)**2
                                                                       DGRS1300
   BND = FN*(TQ(4)*EPS)**2
                                                                       DGRS1310
   EPSOLD = EPS
                                                                       DGRS1320
   NOLD = N
                                                                       DGRS1330
   GO TO (30,35,50), IRET
                                                                       DGRS1340
25 IF ((EPS.EQ.EPSOLD).AND.(N.EQ.NOLD)) GO TO 30
                                                                       DGRS1350
   IF (N.EO.NOLD) IWEVAL = MITER
                                                                       DGRS1360
                                                                       DGRS1370
   IRET = 1
   GO TO 20
                                                                       DGRS1380
30 IF (H.EQ.HOLD) GO TO 50
                                                                       DGRS1390
   RH = H/HOLD
                                                                       DGRS1400
   H = HOLD
                                                                       DGRS1410
   IREDO = 3
                                                                       DGRS1420
   GO TO 40
                                                                       DGRS1430
35 RH = DMAX1 (RH, HMIN/DABS(H))
                                                                       DGRS1440
40 RH = DMIN1 (RH, HMAX/DABS (H), RMAX)
                                                                       DGRS1450
                                                                       DGRS1460
   R1 = 1.D0
                                                                       DGRS1470
   DO 45 J=2, L
                                                                       DGRS1480
      R1 = R1*RH
   DO 45 I=1, N
                                                                       DGRS1490
                                                                       DGRS1500
45 Y(I,J) = Y(I,J)*R1
   H = H*RH
                                                                       DGRS1510
   RC = RC*RH
                                                                       DGRS1520
   IDOUB = L+1
                                                                       DGRS1530
                                                                       DGRS1540
   IF (IREDO.EQ.0) GO TO 285
                                THIS SECTION COMPUTES THE PREDICTED
                                                                       DGRS1550
                                                                       DGRS1560
                                  VALUES BY EFFECTIVELY MULTIPLYING
                                  THE Y ARRAY BY THE PASCAL TRIANGLE DGRS1570
                                  MATRIX. RC IS THE RATIO OF NEW TO
                                                                       DGRS1580
                                  OLD VALUES OF THE COEFFICIENT
                                                                       DGRS1590
                                  H*EL(1). WHEN RC DIFFERS FROM 1 BY DGRS1600
                                  MORE THAN 30 PERCENT, OR THE
                                                                       DGRS1610
                                  CALLER HAS CHANGED MITER, IWEVAL
                                                                       DGRS1620
                                  IS SET TO MITER TO FORCE THE
                                                                       DGRS1630
                                   PARTIALS TO BE UPDATED, IF
                                                                       DGRS1640
                                  PARTIALS ARE USED. IN ANY CASE,
                                                                       DGRS1650
                                  THE PARTIALS ARE UPDATED AT LEAST
                                                                       DGRS1660
                                  EVERY 20-TH STEP.
                                                                       DGRS1670
50 IF (DABS (RC-1.D0).GT.0.3D0) IWEVAL = MITER
                                                                       DGRS1680
   IF (NSTEP.GE.NSTEPJ+20) IWEVAL = MITER
                                                                       DGRS1690
   T = T + H
                                                                       DGRS1700
   DO 55 J1=1, NQ
                                                                       DGRS1710
   DO 55 J2=J1, NO
                                                                       DGRS1720
      J = (NQ+J1)-J2
                                                                       DGRS1730
   DO 55 I=1, N
                                                                       DGRS1740
55 Y(I,J) = Y(I,J) + Y(I,J+1)
                                                                       DGRS1750
                                UP TO 3 CORRECTOR ITERATIONS ARE
                                                                       DGRS1760
                                  TAKEN. A CONVERGENCE TEST IS MADE
                                                                       DGRS1770
                                   ON THE R.M.S. NORM OF EACH
                                                                       DGRS1780
                                   CORRECTION, USING BND, WHICH IS
                                                                       DGRS1790
                                   DEPENDENT ON EPS. THE SUM OF THE
                                  CORRECTIONS IS ACCUMULATED IN THE
                                                                       DGRS1810
                                   VECTOR ERROR(I). THE Y ARRAY IS
                                                                       DGRS1820
                                  NOT ALTERED IN THE CORRECTOR LOOP. DGRS1830
                                  THE UPDATED Y VECTOR IS STORED
                                                                       DGRS1840
```

C

C

C

C

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C

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C
                                      TEMPORARILY IN SAVE1.
                                                                           DGRS1850
   60 DO 65 I=1,N
                                                                            DGRS1860
   65 \text{ ERROR}(I) = 0.D0
                                                                            DGRS1870
                                                                            DGRS1880
      M = 0
      CALL FCN (N,T,Y,SAVE2,eprime,eprime2)
      NFE = NFE+1
                                                                            DGRS1900
      IF (IWEVAL.LE.0) GO TO 95
                                                                            DGRS1910
C
                                    IF INDICATED, THE MATRIX P = I -
                                                                            DGRS1920
C
                                      H*EL(1)*J IS REEVALUATED BEFORE
                                                                            DGRS1930
C
                                      STARTING THE CORRECTOR ITERATION.
                                                                            DGRS1940
C
                                      IWEVAL IS SET TO 0 AS AN INDICATOR DGRS1950
C
                                      THAT THIS HAS BEEN DONE. IF MITER DGRS1960
C
                                      = 1 OR 2, P IS COMPUTED AND
                                                                            DGRS1970
000
                                      PROCESSED IN PSET. IF MITER = 3,
                                                                            DGRS1980
                                      THE MATRIX USED IS P = I -
                                                                            DGRS1990
C
                                      H*EL(1)*D, WHERE D IS A DIAGONAL
                                                                            DGRS2000
                                      MATRIX.
                                                                            DGRS2010
      IWEVAL = 0
                                                                            DGRS2020
      RC = 1.D0
                                                                            DGRS2030
      NJE = NJE+1
                                                                            DGRS2040
      NSTEPJ = NSTEP
                                                                            DGRS2050
      GO TO (75,70,80), MITER
                                                                            DGRS2060
   70 \text{ NFE} = \text{NFE+N}
                                                                            DGRS2070
   75 \text{ CON} = -\text{H*EL}(1)
                                                                            DGRS2080
      MITER1 = MITER
                                                                            DGRS2090
      CALL DGRPS (FCN, FCNJ, Y, NO, CON, MITER1, YMAX, SAVE1, SAVE2, PW, EQUIL,
                                                                           DGRS2100
     1 IPIV, IER)
                                                                            DGRS2110
      IF (IER.NE.0) GO TO 155
                                                                            DGRS2120
      GO TO 125
                                                                            DGRS2130
   80 R = EL(1) * .1D0
                                                                            DGRS2140
      DO 85 I=1,N
                                                                            DGRS2150
   85 PW(I) = Y(I,1) + R*(H*SAVE2(I) - Y(I,2))
                                                                            DGRS2160
      CALL FCN (N,T,PW,SAVE1,eprime,eprime2)
      NFE = NFE+1
                                                                            DGRS2180
      HL0 = H*EL(1)
                                                                            DGRS2190
      DO 90 I=1, N
                                                                            DGRS2200
          R0 = H*SAVE2(I) - Y(I, 2)
                                                                            DGRS2210
          PW(I) = 1.D0
                                                                            DGRS2220
          D = .1D0*R0-H*(SAVE1(I)-SAVE2(I))
                                                                            DGRS2230
          SAVE1(I) = 0.D0
                                                                            DGRS2240
          IF (DABS(R0).LT.UROUND*YMAX(I)) GO TO 90
                                                                            DGRS2250
          IF (DABS(D).EQ.0.D0) GO TO 155
                                                                            DGRS2260
          PW(I) = .1D0*R0/D
                                                                            DGRS2270
          SAVE1(I) = PW(I) *R0
                                                                            DGRS2280
   90 CONTINUE
                                                                            DGRS2290
      GO TO 135
                                                                            DGRS2300
   95 IF (MITER.NE.0) GO TO (125,125,105), MITER
                                                                            DGRS2310
C
                                                                            DGRS2320
C
                                    IN THE CASE OF FUNCTIONAL ITERATION, DGRS2330
С
                                      UPDATE Y DIRECTLY FROM THE RESULT DGRS2340
C
                                       OF THE LAST FCN CALL.
                                                                            DGRS2350
      D = 0.D0
                                                                            DGRS2360
      DO 100 I=1, N
                                                                            DGRS2370
          R = H*SAVE2(I) - Y(I,2)
                                                                            DGRS2380
          D = D + ((R - ERROR(I)) / YMAX(I)) **2
                                                                            DGRS2390
          SAVE1(I) = Y(I,1)+EL(1)*R
                                                                            DGRS2400
  100 \text{ ERROR}(I) = R
                                                                            DGRS2410
       GO TO 145
                                                                            DGRS2420
                                     IN THE CASE OF THE CHORD METHOD,
                                                                            DGRS2430
C
                                       COMPUTE THE CORRECTOR ERROR, F SUB DGRS2440
                                       (M), AND SOLVE THE LINEAR SYSTEM DGRS2450
C
                                      WITH THAT AS RIGHT-HAND SIDE AND P DGRS2460
```

```
AS COEFFICIENT MATRIX, USING THE
                                                                              DGRS2470
C
                                       LU DECOMPOSITION IF MITER = 1 OR 2. IF MITER = 3, THE COEFFICIENT
C
                                                                              DGRS2480
C
                                                                              DGRS2490
                                       H*EL(1) IN P IS UPDATED.
                                                                              DGRS2500
  105 \text{ PHLO} = \text{HLO}
                                                                              DGRS2510
      HL0 = H*EL(1)
                                                                              DGRS2520
      IF (HLO.EQ.PHLO) GO TO 115
                                                                              DGRS2530
      R = HL0/PHL0
                                                                              DGRS2540
      DO 110 I=1, N
                                                                              DGRS2550
         D = 1.D0-R*(1.D0-1.D0/PW(I))
                                                                              DGRS2560
          IF (DABS(D).EO.O.DO) GO TO 165
                                                                              DGRS2570
  110 \text{ PW}(I) = 1.\text{DO/D}
                                                                              DGRS2580
  115 DO 120 I=1, N
                                                                              DGRS2590
  120 SAVE1(I) = PW(I) * (H*SAVE2(I) - (Y(I, 2) + ERROR(I)))
                                                                              DGRS2600
                                                                              DGRS2610
      GO TO 135
  125 DO 130 I=1, N
                                                                              DGRS2620
  130 SAVE1(I) = H*SAVE2(I) - (Y(I,2) + ERROR(I))
                                                                              DGRS2630
      IF (NLC .EO. -1) GO TO 131
                                                                              DGRS2640
      NWK = (NLC+NUC+1)*NO+1
                                                                              DGRS2650
      CALL LEQT1B (PW, N, NLC, NUC, NO, SAVE1, 1, NO, 2, PW (NWK), JER)
                                                                              DGRS2660
                                                                              DGRS2670
      GO TO 135
  131 CALL LUELMF (PW. SAVE1. IPIV. N. NO. SAVE1)
                                                                              DGRS2680
                                                                              DGRS2690
  135 D = 0.D0
      DO 140 I=1, N
                                                                              DGRS2700
          ERROR(I) = ERROR(I) + SAVE1(I)
                                                                              DGRS2710
          D = D + (SAVE1(I)/YMAX(I)) **2
                                                                              DGRS2720
  140 SAVE1(I) = Y(I,1) + EL(1) * ERROR(I)
                                                                              DGRS2730
                                     TEST FOR CONVERGENCE. IF M.GT.O, THE DGRS2740
CCC
                                        SQUARE OF THE CONVERGENCE RATE
                                                                              DGRS2750
                                        CONSTANT IS ESTIMATED AS CRATE,
                                                                              DGRS2760
C
                                                                              DGRS2770
                                        AND THIS IS USED IN THE TEST.
  145 IF (M.NE.O) CRATE = DMAX1 (.9D0*CRATE, D/D1)
                                                                              DGRS2780
      IF ((D*DMIN1(1.D0,2.D0*CRATE)).LE.BND) GO TO 170
                                                                              DGRS2790
      D1 = D
                                                                              DGRS2800
      M = M+1
                                                                              DGRS2810
                                                                              DGRS2820
      IF (M.EQ.3) GO TO 150
      CALL FCN (N,T,SAVE1,SAVE2,eprime,eprime2)
                                                                                +
                                                                              DGRS2840
C
                                     THE CORRECTOR ITERATION FAILED TO
                                                                              DGRS2850
000000
                                        CONVERGE IN 3 TRIES. IF PARTIALS
                                                                              DGRS2860
                                        ARE INVOLVED BUT ARE NOT UP TO
                                                                              DGRS2870
                                        DATE, THEY ARE REEVALUATED FOR THE DGRS2880
                                        NEXT TRY. OTHERWISE THE Y ARRAY IS DGRS2890
                                        RETRACTED TO ITS VALUES BEFORE
                                                                              DGRS2900
                                        PREDICTION, AND H IS REDUCED, IF
                                                                              DGRS2910
C
                                        POSSIBLE. IF NOT, A NO-CONVERGENCE DGRS2920
                                        EXIT IS TAKEN.
                                                                              DGRS2930
  150 \text{ NFE} = \text{NFE}+2
                                                                              DGRS2940
       IF (IWEVAL.EQ.-1) GO TO 165
                                                                              DGRS2950
  155 T = TOLD
                                                                              DGRS2960
       RMAX = 2.D0
                                                                              DGRS2970
       DO 160 J1=1,NQ
                                                                              DGRS2980
       DO 160 J2=J1, NQ
                                                                              DGRS2990
          J = (NQ+J1)-J2
                                                                              DGRS3000
       DO 160 I=1, N
                                                                               DGRS3010
  160 Y(I,J) = Y(I,J) - Y(I,J+1)
                                                                               DGRS3020
       IF (DABS(H).LE.HMIN*1.00001D0) GO TO 280
                                                                               DGRS3030
       RH = .25D0
                                                                               DGRS3040
       IREDO = 1
                                                                               DGRS3050
       GO TO 35
                                                                               DGRS3060
  165 IWFVAL = MITER
                                                                               DGRS3070
       GO'TO 60
                                                                               DGRS3080
```

```
C
                                   THE CORRECTOR HAS CONVERGED. IWEVAL
                                                                          DGRS3090
C
                                      IS SET TO -1 IF PARTIAL
                                                                           DGRS3100
C
                                     DERIVATIVES WERE USED, TO SIGNAL
                                                                           DGRS3110
                                     THAT THEY MAY NEED UPDATING ON
                                                                           DGRS3120
C
                                     SUBSEQUENT STEPS. THE ERROR TEST
                                                                           DGRS3130
C
                                      IS MADE AND CONTROL PASSES TO
                                                                           DGRS3140
C
                                      STATEMENT 190 IF IT FAILS.
                                                                           DGRS3150
  170 IF (MITER.NE.0) IWEVAL = -1
                                                                           DGRS3160
      NFE = NFE+M
                                                                           DGRS3170
      D = 0.D0
                                                                           DGRS3180
      DO 175 I=1, N
                                                                           DGRS3190
  175 D = D+(ERROR(I)/YMAX(I))**2
                                                                           DGRS3200
      IF (D.GT.E) GO TO 190
                                                                           DGRS3210
C
                                   AFTER A SUCCESSFUL STEP, UPDATE THE
                                                                           DGRS3220
C
                                      Y ARRAY. CONSIDER CHANGING H IF
                                                                           DGRS3230
C
                                      IDOUB = 1. OTHERWISE DECREASE
                                                                           DGRS3240
C
                                      IDOUB BY 1. IF IDOUB IS THEN 1 AND DGRS3250
CCC
                                      NQ .LT. MAXDER, THEN ERROR IS
                                                                           DGRS3260
                                      SAVED FOR USE IN A POSSIBLE ORDER
                                                                           DGRS3270
                                      INCREASE ON THE NEXT STEP. IF A
                                                                           DGRS3280
C
                                      CHANGE IN H IS CONSIDERED, AN
                                                                           DGRS3290
C
                                      INCREASE OR DECREASE IN ORDER BY
                                                                           DGRS3300
C
                                      ONE IS CONSIDERED ALSO. A CHANGE
                                                                           DGRS3310
C
                                      IN H IS MADE ONLY IF IT IS BY A
                                                                           DGRS3320
C
                                      FACTOR OF AT LEAST 1.1. IF NOT,
                                                                           DGRS3330
                                      IDOUB IS SET TO 10 TO PREVENT
C
                                                                           DGRS3340
C
                                      TESTING FOR THAT MANY STEPS.
                                                                           DGRS3350
      KFLAG = 0
                                                                           DGRS3360
      IREDO = 0
                                                                           DGRS3370
      NSTEP = NSTEP+1
                                                                           DGRS3380
      HUSED = H
                                                                           DGRS3390
      NOUSED = NO
                                                                           DGRS3400
      DO 180 J=1,L
                                                                           DGRS3410
      DO 180 I=1,N
                                                                           DGRS3420
  180 Y(I,J) = Y(I,J) + EL(J) * ERROR(I)
                                                                           DGRS3430
      IF (IDOUB.EQ.1) GO TO 200
                                                                           DGRS3440
      IDOUB = IDOUB-1
                                                                           DGRS3450
      IF (IDOUB.GT.1) GO TO 290
                                                                           DGRS3460
      IF (L.EQ.LMAX) GO TO 290
                                                                           DGRS3470
      DO 185 I=1,N
                                                                           DGRS3480
  185 \text{ Y}(I, LMAX) = ERROR(I)
                                                                           DGRS3490
      GO TO 290
                                                                           DGRS3500
C
                                    THE ERROR TEST FAILED. KFLAG KEEPS
                                                                           DGRS3510
C
                                      TRACK OF MULTIPLE FAILURES.
                                                                           DGRS3520
C C C
                                      RESTORE T AND THE Y ARRAY TO THEIR DGRS3530
                                      PREVIOUS VALUES, AND PREPARE TO
                                                                           DGRS3540
                                      TRY THE STEP AGAIN. COMPUTE THE
                                                                           DGRS3550
                                      OPTIMUM STEP SIZE FOR THIS OR ONE
                                                                           DGRS3560
                                      LOWER ORDER.
                                                                           DGRS3570
  190 KFLAG = KFLAG-1
                                                                           DGRS3580
      T = TOLD
                                                                           DGRS3590
      DO 195 J1=1, NQ
                                                                           DGRS3600
      DO 195 J2=J1, NO
                                                                           DGRS3610
          J = (NQ+J1)-J2
                                                                           DGRS3620
      DO 195 I=1, N
                                                                           DGRS3630
  195 Y(I,J) = Y(I,J) - Y(I,J+1)
                                                                           DGRS3640
      RMAX = 2.D0
                                                                           DGRS3650
      IF (DABS(H).LE.HMIN*1.00001D0) GO TO 270
                                                                           DGRS3660
      IF (KFLAG.LE.-3) GO TO 260
                                                                           DGRS3670
      IREDO = 2
                                                                           DGRS3680
      PR3 = 1.D+20
                                                                           DGRS3690
      GO TO 210
                                                                           DGRS3700
```

```
REGARDLESS OF THE SUCCESS OR FAILURE DGRS3710
                                      OF THE STEP, FACTORS PR1, PR2, AND DGRS3720
0000000000
                                      PR3 ARE COMPUTED, BY WHICH H COULD DGRS3730
                                      BE DIVIDED AT ORDER NQ - 1, ORDER DGRS3740
                                      NQ, OR ORDER NQ + 1, RESPECTIVELY. DGRS3750
                                       IN THE CASE OF FAILURE, PR3 =
                                                                             DGRS3760
                                       1.E20 TO AVOID AN ORDER INCREASE.
                                                                             DGRS3770
                                       THE SMALLEST OF THESE IS
                                                                             DGRS3780
                                       DETERMINED AND THE NEW ORDER
                                                                             DGRS3790
                                      CHOSEN ACCORDINGLY. IF THE ORDER
                                                                             DGRS3800
                                      IS TO BE INCREASED, WE COMPUTE ONE DGRS3810
                                      ADDITIONAL SCALED DERIVATIVE.
                                                                             DGRS3820
  200 \text{ PR3} = 1.D+20
                                                                             DGRS3830
      IF (L.EO.LMAX) GO TO 210
                                                                             DGRS3840
                                                                             DGRS3850
      D1 = 0.D0
      DO 205 I=1, N
                                                                             DGRS3860
  205 D1 = D1 + ((ERROR(I) - Y(I, LMAX)) / YMAX(I)) **2
                                                                             DGRS3870
      ENQ3 = .5D0/(L+1)
                                                                             DGRS3880
      PR3 = ((D1/EUP) **ENQ3) *1.4D0+1.4D-6
                                                                             DGRS3890
  210 \text{ ENO2} = .5\text{D0/L}
                                                                             DGRS3900
      PR2 = ((D/E) **ENQ2) *1.2D0+1.2D-6
                                                                             DGRS3910
      PR1 = 1.D+20
                                                                             DGRS3920
      IF (NQ.EQ.1) GO TO 220
                                                                             DGRS3930
      D = 0.D0
                                                                             DGRS3940
                                                                             DGRS3950
      DO 215 I=1, N
  215 D = D + (Y(I, L) / YMAX(I)) **2
                                                                             DGRS3960
      ENO1 = .5D0/NQ
                                                                             DGRS3970
      PR1 = ((D/EDN) **ENQ1) *1.3D0+1.3D-6
                                                                             DGRS3980
  220 IF (PR2.LE.PR3) GO TO 225
                                                                             DGRS3990
      IF (PR3.LT.PR1) GO TO 235
                                                                             DGRS4000
      GO TO 230
                                                                             DGRS4010
  225 IF (PR2.GT.PR1) GO TO 230
                                                                             DGRS4020
      NEWQ = NQ
                                                                             DGRS4030
      RH = 1.D0/PR2
                                                                             DGRS4040
      GO TO 250
                                                                             DGRS4050
  230 \text{ NEWQ} = \text{NQ-1}
                                                                             DGRS4060
      RH = 1.D0/PR1
                                                                             DGRS4070
      IF (KFLAG.NE.O.AND.RH.GT.1.DO) RH = 1.DO
                                                                             DGRS4080
      GO TO 250
                                                                             DGRS4090
  235 \text{ NEWO} = L
                                                                             DGRS4100
      RH = 1.D0/PR3
                                                                             DGRS4110
      IF (RH.LT.1.1D0) GO TO 245
                                                                             DGRS4120
      DO 240 I=1, N
                                                                             DGRS4130
  240 Y(I, NEWO+1) = ERROR(I) *EL(L)/L
                                                                             DGRS4140
      GO TO 255
                                                                             DGRS4150
  245 \text{ IDOUB} = 10
                                                                             DGRS4160
      GO TO 290
                                                                             DGRS4170
  250 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1D0)) GO TO 245
                                                                             DGRS4180
C
                                                                             DGRS4190
C
                                     IF THERE IS A CHANGE OF ORDER, RESET DGRS4200
C
                                       NO, L, AND THE COEFFICIENTS. IN
                                                                             DGRS4210
C
                                       ANY CASE H IS RESET ACCORDING TO
                                                                             DGRS4220
C
                                       RH AND THE Y ARRAY IS RESCALED.
                                                                             DGRS4230
C
                                       THEN EXIT FROM 285 IF THE STEP WAS DGRS4240
                                       OK, OR REDO THE STEP OTHERWISE.
                                                                             DGRS4250
      IF (NEWO.EO.NO) GO TO 35
                                                                             DGRS4260
  255 \text{ NO} = \text{NEWO}
                                                                             DGRS4270
      L = NO+1
                                                                             DGRS4280
      IRET = 2
                                                                             DGRS4290
      GO TO 15
                                                                             DGRS4300
C
                                     CONTROL REACHES THIS SECTION IF 3 OR DGRS4310
C
                                       MORE FAILURES HAVE OCCURED. IT IS DGRS4320
```

```
ASSUMED THAT THE DERIVATIVES THAT
C
                                                                              DGRS4330
00000000
                                       HAVE ACCUMULATED IN THE Y ARRAY
                                                                              DGRS4340
                                       HAVE ERRORS OF THE WRONG ORDER.
                                                                              DGRS4350
                                       HENCE THE FIRST DERIVATIVE IS
                                                                              DGRS4360
                                       RECOMPUTED, AND THE ORDER IS SET
                                                                              DGRS4370
                                       TO 1. THEN H IS REDUCED BY A
                                                                              DGRS4380
                                       FACTOR OF 10, AND THE STEP IS
                                                                              DGRS4390
                                       RETRIED. AFTER A TOTAL OF 7
                                                                              DGRS4400
                                       FAILURES, AN EXIT IS TAKEN WITH
                                                                              DGRS4410
C
                                       KFLAG = -2.
                                                                              DGRS4420
  260 IF (KFLAG.EQ.-7) GO TO 275
                                                                              DGRS4430
      RH = .1D0
                                                                              DGRS4440
      RH = DMAX1(HMIN/DABS(H), RH)
                                                                              DGRS4450
      H = H*RH
                                                                              DGRS4460
      CALL FCN (N,T,Y,SAVE1,eprime,eprime2)
      NFE = NFE+1
                                                                              DGRS4480
      DO 265 I=1,N
                                                                              DGRS4490
  265 Y(I,2) = H*SAVE1(I)
                                                                              DGRS4500
      IWEVAL = MITER
                                                                              DGRS4510
      IDOUB = 10
                                                                              DGRS4520
      IF (NQ.EQ.1) GO TO 50
                                                                              DGRS4530
      NQ = 1
                                                                              DGRS4540
      L = 2
                                                                              DGRS4550
      IRET = 3
                                                                              DGRS4560
      GO TO 15
                                                                              DGRS4570
C
                                     ALL RETURNS ARE MADE THROUGH THIS
                                                                              DGRS4580
CCC
                                       SECTION. H IS SAVED IN HOLD TO
                                                                              DGRS4590
                                       ALLOW THE CALLER TO CHANGE H ON
                                                                              DGRS4600
                                        THE NEXT STEP.
                                                                              DGRS4610
                                                                              DGRS4620
  270 \text{ KFLAG} = -1
      GO TO 290
                                                                              DGRS4630
  275 \text{ KFLAG} = -2
                                                                              DGRS4640
      GO TO 290
                                                                              DGRS4650
  280 \text{ KFLAG} = -3
                                                                              DGRS4660
       GO TO 290
                                                                              DGRS4670
  285 \text{ RMAX} = 10.D0
                                                                              DGRS4680
  290 \text{ HOLD} = H
                                                                              DGRS4690
      JSTART = NQ
                                                                              DGRS4700
C--Diagnostic Check of first and second derivatives of E
                                                                                +
       if (tcum.eq.told) go to 310
                                                                                 +
       write (8,300) tcum, step, y(1,1), y(2,1), y(3,1), y(4,1), y(5,1)
                                                                                 +
  300 format(1x,e11.4,1x,I5,5(1x,e11.4))
                                                                                 +
       write (9,305) step, eprime, eprime2
                                                                                 +
  305 format(1x, I5, 2(1x, e20.13))
       RETURN
                                                                              DGRS4710
       END
                                                                              DGRS4720
```

```
IMSL ROUTINE NAME - DGRCS
                                                                      DGRC0010
C
                                                                      DGRC0020
C
         C- -
C
                                                                      DGRC0040
C
   COMPUTER
                       - IBM/DOUBLE
                                                                      DGRC0050
C
                                                                      DGRC0060
C
   LATEST REVISION
                      - JANUARY 1, 1978
                                                                      DGRC0070
C
                                                                      DGRC0080
C
   PURPOSE
                       - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR DGRC0090
C
                                                                      DGRC0100
   PRECISION/HARDWARE - SINGLE AND DOUBLE/H32
C
                                                                      DGRC0110
                       - SINGLE/H36, H48, H60
C
                                                                      DGRC0120
C
                                                                      DGRC0130
C
   REOD. IMSL ROUTINES - NONE REQUIRED
                                                                      DGRC0140
C
                                                                      DGRC0150
C
   NOTATION
                       - INFORMATION ON SPECIAL NOTATION AND
                                                                      DGRC0160
C
                          CONVENTIONS IS AVAILABLE IN THE MANUAL
                                                                      DGRC0170
                          INTRODUCTION OR THROUGH IMSL ROUTINE UHELP DGRC0180
C
C
                                                                      DGRC0190
  COPYRIGHT
                      - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.
C
                                                                      DGRC0200
C
                                                                      DGRC0210
                      - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN DGRC0220
C
   WARRANTY
C
                          APPLIED TO THIS CODE. NO OTHER WARRANTY,
                                                                      DGRC0230
C
                          EXPRESSED OR IMPLIED, IS APPLICABLE.
                                                                      DGRC0240
C
                                                                      DGRC0250
C--
                         ---------DGRC0260
C
                                                                      DGRC0270
     SUBROUTINE DGRCS (METH, NQ, EL, TQ, MAXDER)
                                                                      DGRC0280
                                 SPECIFICATIONS FOR ARGUMENTS
C
                                                                      DGRC0290
     INTEGER
                        METH, NQ, MAXDER
                                                                      DGRC0300
      REAL
                        TO(1)
                                                                      DGRC0310
     DOUBLE PRECISION
                        EL(1)
                                                                      DGRC0320
                                 SPECIFICATIONS FOR LOCAL VARIABLES
                                                                      DGRC0330
C
      INTEGER
                                                                      DGRC0340
                        PERTST(12,2,3)
      REAL
                                                                      DGRC0350
     DATA
                       PERTST/1.,1.,2.,1.,.3158,.7407E-1,
                                                                      DGRC0360
                                                                     DGRC0370
                       .1391E-1,.2182E-2,.2945E-3,.3492E-4,
    1
                       .3692E-5,.3524E-6,1.,1.,.5,.1667,
     2
                                                                      DGRC0380
     3
                        .4167E-1,7*1.,2.,12.,24.,37.89,
                                                                      DGRC0390
                        53.33,70.08,87.97,106.9,126.7,
                                                                     DGRC0400
     4
                        147.4,168.8,191.0,2.0,4.5,7.333,
                                                                     DGRC0410
     5
                        10.42,13.7,7*1.,12.0,24.0,37.89,
                                                                     DGRC0420
     6
     7
                        53.33,70.08,87.97,106.9,126.7,
                                                                      DGRC0430
     8
                        147.4,168.8,191.0,1.,3.0,6.0,
                                                                      DGRC0440
                        9.167,12.5,8*1./
                                                                      DGRC0450
                                FIRST EXECUTABLE STATEMENT
                                                                      DGRC0460
C
     GO TO (5,10), METH
                                                                      DGRC0470
    5 MAXDER = 12
                                                                      DGRC0480
      GO TO (15,20,25,30,35,40,45,50,55,60,65,70), NQ
                                                                      DGRC0490
   10 MAXDER = 5
                                                                      DGRC0500
      GO TO (75,80,85,90,95), NQ
                                                                      DGRC0510
                                 THE FOLLOWING COEFFICIENTS SHOULD BE DGRC0520
C
C
                                   DEFINED TO MACHINE ACCURACY. FOR A DGRC0530
C
                                    GIVEN ORDER NQ, THEY CAN BE DGRC0540
C
                                    CALCULATED BY USE OF THE
                                                                      DGRC0550
C
                                   GENERATING POLYNOMIAL L(T), WHOSE DGRC0560
                                   COEFFICIENTS ARE EL(I).. L(T) = DGRC0570
C
C
                                    EL(1) + EL(2)*T + ... +
                                                                      DGRC0580
                                   EL(NQ+1)*T**NQ. FOR THE IMPLICIT DGRC0590
ADAMS METHODS, L(T) IS GIVEN BY DGRC0600
DL/DT = (T+1)*(T+2)* ... DGRC0610
C
C
C
                                   *(T+NQ-1)/K, L(-1) = 0, WHERE K = DGRC0620
```

| C     |                                    | FACTORIAL (NQ-1). FOR THE GEAR        | DGRC0630 |
|-------|------------------------------------|---------------------------------------|----------|
| C     |                                    | METHODS, $L(T) = (T+1)*(T+2)*$        | DGRC0640 |
| C     |                                    | *(T+NQ)/K, WHERE $K =$                | DGRC0650 |
| C     |                                    | FACTORIAL (NQ) * $(1 + 1/2 + \dots +$ | DGRC0660 |
| С     |                                    | 1/NQ). THE ORDER IN WHICH THE         | DGRC0670 |
| 00000 |                                    | GROUPS APPEAR BELOW IS IMPLICIT       | DGRC0680 |
| C     |                                    | ADAMS METHODS OF ORDERS 1 TO 12,      | DGRC0690 |
| C     |                                    | BACKWARD DIFFERENTIATION METHODS      | DGRC0700 |
| С     |                                    | OF ORDERS 1 TO 5.                     | DGRC0710 |
|       | 15 EL(1) = 1.0D0                   |                                       | DGRC0720 |
|       | GO TO 100                          |                                       | DGRC0730 |
|       | 20  EL(1) = 0.5D0                  |                                       | DGRC0740 |
|       | EL(3) = 0.5D0                      |                                       | DGRC0750 |
|       | GO TO 100                          |                                       | DGRC0760 |
|       | 25  EL(1) = 4.166666666666667D-01  |                                       | DGRC0770 |
|       | EL(3) = 0.75D0                     |                                       | DGRC0780 |
|       | EL(4) = 1.66666666666667D-01       |                                       | DGRC0790 |
|       | GO TO 100                          |                                       | DGRC0800 |
|       | 30  EL(1) = 0.375D0                |                                       | DGRC0810 |
|       | EL(3) = 9.16666666666667D-01       |                                       | DGRC0820 |
|       | EL(4) = 3.33333333333333330-01     |                                       | DGRC0830 |
|       | EL(5) = 4.166666666666667D-02      |                                       | DGRC0840 |
|       | GO TO 100                          |                                       | DGRC0850 |
|       | 35  EL(1) = 3.4861111111111111D-01 |                                       | DGRC0860 |
|       | EL(3) = 1.041666666666667D0        |                                       | DGRC0870 |
|       | EL(4) = 4.8611111111111110-01      |                                       | DGRC0880 |
|       | EL(5) = 1.041666666666667D-03      |                                       | DGRC0890 |
|       | EL(6) = 8.33333333333333330-03     | 3                                     | DGRC0900 |
|       | GO TO 100                          |                                       | DGRC0910 |
|       | 40  EL(1) = 3.2986111111111111D-01 |                                       | DGRC0920 |
|       | EL(3) = 1.141666666666667D+00      | )                                     | DGRC0930 |
|       | EL(4) = 0.625D+00                  |                                       | DGRC0940 |
|       | EL(5) = 1.7708333333333333D-03     |                                       | DGRC0950 |
|       | EL(6) = 0.025D+00                  |                                       | DGRC0960 |
|       | EL(7) = 1.38888888888889D-03       | 3                                     | DGRC0970 |
|       | GO TO 100                          |                                       | DGRC0980 |
|       | 45  EL(1) = 3.155919312169312D-03  | L                                     | DGRC0990 |
|       | EL(3) = 1.225D+00                  |                                       | DGRC1000 |
|       | EL(4) = 7.518518518518519D-03      | 1                                     | DGRC1010 |
|       | EL(5) = 2.5520833333333333D-03     | 1                                     | DGRC1020 |
|       | EL(6) = 4.8611111111111111D-03     | 2                                     | DGRC1030 |
|       | EL(7) = 4.8611111111111111D-0      |                                       | DGRC1040 |
|       | EL(8) = 1.984126984126984D - 04    | 4                                     | DGRC1050 |
|       | GO TO 100                          |                                       | DGRC1060 |
|       | 50  EL(1) = 3.042245370370370D-03  |                                       | DGRC1070 |
|       | EL(3) = 1.296428571428571D+0       | 0                                     | DGRC1080 |
|       | EL(4) = 8.685185185185185D-0       |                                       | DGRC1090 |
|       | EL(5) = 3.357638888888889D-0       | 1                                     | DGRC1100 |
|       | EL(6) = 7.77777777777778D-03       | 2                                     | DGRC1110 |
|       | EL(7) = 1.064814814814815D-03      | 2                                     | DGRC1120 |
|       | EL(8) = 7.936507936507937D-04      | 4                                     | DGRC1130 |
|       | EL(9) = 2.480158730158730D-09      |                                       | DGRC1140 |
|       | GO TO 100                          |                                       | DGRC1150 |
|       | 55  EL(1) = 2.948680004409171D-03  | 1                                     | DGRC1160 |
|       | EL(3) = 1.358928571428571D+0       | 0                                     | DGRC1170 |
|       | EL(4) = 9.765542328042328D-0       | 1                                     | DGRC1180 |
|       | EL(5) = 4.171875D-01               |                                       | DGRC1190 |
|       | EL(6) = 1.113541666666667D-0       | 1                                     | DGRC1200 |
|       | EL(7) = 0.01875D+00                |                                       | DGRC1210 |
|       | EL(8) = 1.934523809523810D-0       | 3                                     | DGRC1220 |
|       | EL(9) = 1.116071428571429D-0       | 4                                     | DGRC1230 |
|       | EL(10) = 2.755731922398589D-0      | 6                                     | DGRC1240 |
|       |                                    |                                       |          |

|   |     | GO TO 100                               | DGRC1250 |
|---|-----|---|----------|
|   | 60  | EL(1) = 2.869754464285714D-01           | DGRC1260 |
|   | 00  | EL(3) = 1.414484126984127D+00           | DGRC1270 |
|   |     | EL(4) = 1.077215608465609D+00           | DGRC1270 |
|   |     | , ,                                     |          |
|   |     | EL(5) = 4.985670194003527D-01           | DGRC1290 |
|   |     | EL(6) = 1.484375D-01                    | DGRC1300 |
|   |     | EL(7) = 2.906057098765432D-02           | DGRC1310 |
|   |     | EL(8) = 3.720238095238095D-03           | DGRC1320 |
|   |     | EL(9) = 2.996858465608466D-04           | DGRC1330 |
|   |     | EL(10) = 1.377865961199295D-05          | DGRC1340 |
|   |     | EL(11) = 2.755731922398589D-07          | DGRC1350 |
|   |     | GO TO 100                               | DGRC1360 |
|   | 65  | EL(1) = 2.801895964439367D-01           | DGRC1370 |
|   | 0.5 | EL(3) = 1.464484126984127D+00           | DGRC1370 |
|   |     |   |          |
|   |     | EL(4) = 1.171514550264550D+00           | DGRC1390 |
|   |     | EL(5) = 5.793581900352734D-01           | DGRC1400 |
|   |     | EL(6) = 1.883228615520282D-01           | DGRC1410 |
|   |     | EL(7) = 4.143036265432099D-02           | DGRC1420 |
|   |     | EL(8) = 6.211144179894180D-03           | DGRC1430 |
|   |     | EL(9) = 6.252066798941799D-04           | DGRC1440 |
|   |     | EL(10) = 4.041740152851264D-05          | DGRC1450 |
|   |     | EL(11) = 1.515652557319224D-06          | DGRC1460 |
|   |     | EL(12) = 2.505210838544172D-08          | DGRC1470 |
|   |     | GO TO 100                               | DGRC1470 |
|   | 7.0 |   |          |
|   | /0  | EL(1) = 2.742655400315991D-01           | DGRC1490 |
|   |     | EL(3) = 1.509938672438672D+00           | DGRC1500 |
|   |     | EL(4) = 1.260271164021164D+00           | DGRC1510 |
|   |     | EL(5) = 6.592341820987654D-01           | DGRC1520 |
|   |     | EL(6) = 2.304580026455027D-01           | DGRC1530 |
|   |     | EL(7) = 5.569724610523222D-02           | DGRC1540 |
|   |     | EL(8) = 9.439484126984127D-03           | DGRC1550 |
|   |     | EL(9) = 1.119274966931217D-03           | DGRC1560 |
|   |     | EL(10) = 9.093915343915344D-05          | DGRC1570 |
|   |     | EL(11) = 4.822530864197531D-06          | DGRC1570 |
|   |     |   | -        |
|   |     | EL(12) = 1.503126503126503D-07          | DGRC1590 |
|   |     | EL(13) = 2.087675698786810D-09          | DGRC1600 |
|   |     | GO TO 100                               | DGRC1610 |
| C |     |   | DGRC1620 |
|   | 75  | EL(1) = 1.0D+00                         | DGRC1630 |
|   |     | GO TO 100                               | DGRC1640 |
|   | 80  | EL(1) = 6.66666666666667D-01            | DGRC1650 |
|   |     | EL(3) = 3.33333333333333330-01          | DGRC1660 |
|   |     | GO TO 100                               | DGRC1670 |
|   | 85  | EL(1) = 5.4545454545455D-01             | DGRC1680 |
|   |     | EL(3) = EL(1)                           | DGRC1690 |
|   |     | EL(4) = 9.090909090909091D-02           |          |
|   |     |   | DGRC1700 |
|   | 0.0 | GO TO 100                               | DGRC1710 |
|   | 90  | EL(1) = 0.48D+00                        | DGRC1720 |
|   |     | EL(3) = 0.7D+00                         | DGRC1730 |
|   |     | EL(4) = 0.2D+00                         | DGRC1740 |
|   |     | EL(5) = 0.02D+00                        | DGRC1750 |
|   |     | GO TO 100                               | DGRC1760 |
|   | 95  | EL(1) = 4.379562043795620D-01           | DGRC1770 |
|   |     | EL(3) = 8.211678832116788D-01           | DGRC1780 |
|   |     | EL(4) = 3.102189781021898D-01           | DGRC1790 |
|   |     | EL(5) = 5.474452554744526D-02           | DGRC1750 |
|   |     | EL(6) = 3.649635036496350D-03           |          |
| C |     | CO-COCOCOCOCOCOCOCOCOCOCOCOCOCOCOCOCOCO | DGRC1810 |
| _ | 100 | DO 105 K 1 3                            | DGRC1820 |
|   | 100 | DO 105 K=1,3                            | DGRC1830 |
|   |     | TQ(K) = PERTST(NQ, METH, K)             | DGRC1840 |
|   | 105 | CONTINUE                                | DGRC1850 |
|   |     | TQ(4) = .5D0*TQ(2) / (NQ+2)             | DGRC1860 |
|   |     |   |          |

| IMSL ROUTINE NAME   | - DGRPS  | DGRP0010             |
|---------------------|--|----------------------|
|                     |  | DGRP0020             |
|                     |  | -DGRP0030            |
|                     |  | DGRP0040             |
| COMPUTER            | - IBM/DOUBLE   | DGRP0050             |
|                     |  | DGRP0060             |
| LATEST REVISION     | - NOVEMBER 1, 1984   | DGRP0070             |
|                     |  | DGRP0080             |
| PURPOSE             | - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR   |                      |
|                     | GINGI DAND DOITH DAND  | DGRP0100             |
| PRECISION/HARDWARE  | - SINGLE AND DOUBLE/H32  | DGRP0110             |
|                     | - SINGLE/H36,H48,H60   | DGRP0120<br>DGRP0130 |
| DEOD IMCI BOIEFINES | - LUDATF, LEQT1B, UERTST, UGETIO   | DGRP0130             |
| REQD. IMSL ROUTINES | - HODAIF, HEQIID, OERISI, OGEIIO   | DGRP0140             |
| NOTATION            | - INFORMATION ON SPECIAL NOTATION AND  | DGRP0160             |
| HOTATION            | CONVENTIONS IS AVAILABLE IN THE MANUAL   | DGRP0170             |
|                     | INTRODUCTION OR THROUGH IMSL ROUTINE UHELP   | DGRP0180             |
|                     | In the second se | DGRP0190             |
| COPYRIGHT           | - 1984 BY IMSL, INC. ALL RIGHTS RESERVED.  | DGRP0200             |
|                     |  | DGRP0210             |
| WARRANTY            | - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN  | DGRP0220             |
|                     | APPLIED TO THIS CODE. NO OTHER WARRANTY,   | DGRP0230             |
|                     | EXPRESSED OR IMPLIED, IS APPLICABLE.   | DGRP0240             |
|                     |  | DGRP0250             |
|                     |  | -DGRP0260            |
|                     |  | DGRP0270             |
| SUBROUTINE DGRPS    |  | DGRP0280             |
| *                   | EQUIL, IPIV, IER)  | DGRP0290             |
|                     | SPECIFICATIONS FOR ARGUMENTS   | DGRP0300             |
| INTEGER             | NO, MITER, IPIV(1), IER  | DGRP0310             |
| DOUBLE PRECISION    |  |                      |
| *                   | EQUIL(1) SPECIFICATIONS FOR LOCAL VARIABLES  | DGRP0330<br>DGRP0340 |
|                     | SPECIFICATIONS FOR LOCAL VARIABLES   | DGRP0340             |
| INTEGER             | NC, MFC, KFLAG, JSTART, NQUSED, NSTEP, NFE, NJE, NPW,  |                      |
| *                   | NSO, I, J1, J, NERROR, NSAVE1, NSAVE2, NEQUIL, NY,   | DGRP0370             |
| *                   | IDUMMY (23), NLIM, II, IJ, LIM1, LIM2, NB, NLC, NUC, NWK   |                      |
| REAL                | SDUMMY (4)   | DGRP0390             |
| DOUBLE PRECISION    | T, H, HMIN, HMAX, EPSC, UROUND, EPSJ, HUSED, D, RO, YJ, R  | ,DGRP0400            |
| *                   | D1, D2, WA, DUMMY (40)   | DGRP0410             |
| COMMON /DBAND/      | NLC, NUC   | DGRP0420             |
| COMMON /GEAR/       | T, H, HMIN, HMAX, EPSC, UROUND, EPSJ, HUSED, DUMMY,  | DGRP0430             |
| *                   | SDUMMY, NC, MFC, KFLAG, JSTART, NSQ, NQUSED, NSTEP,  | DGRP0440             |
| *                   | NFE, NJE, NPW, NERROR, NSAVE1, NSAVE2, NEQUIL, NY,   | DGRP0450             |
| *                   | IDUMMY   | DGRP0460             |
|                     | THIS ROUTINE IS CALLED BY DGRST TO   | DGRP0470             |
|                     | COMPUTE AND PROCESS THE MATRIX P =   |                      |
|                     | I - H*EL(1)*J , WHERE J IS AN  | DGRP0490             |
|                     | APPROXIMATION TO THE JACOBIAN. J   | DGRP0500             |
|                     | IS COMPUTED, EITHER BY THE USER-<br>SUPPLIED ROUTINE FCNJ IF MITER =   | DGRP0510<br>DGRP0520 |
|                     | 1, OR BY FINITE DIFFERENCING IF  | DGRP0520<br>DGRP0530 |
|                     | MITER = 2. J IS STORED IN PW AND   | DGRP0530             |
|                     | REPLACED BY P, USING CON =   | DGRP0550             |
|                     | -H*EL(1). THEN P IS SUBJECTED TO   | DGRP0560             |
|                     | LU DECOMPOSITION IN PREPARATION  | DGRP0570             |
|                     | FOR LATER SOLUTION OF LINEAR   | DGRP0580             |
|                     | SYSTEMS WITH P AS COEFFICIENT  | DGRP0590             |
|                     | MATRIX. IN ADDITION TO VARIABLES   | DGRP0600             |
|                     | DESCRIBED PREVIOUSLY,  | DGRP0610             |
|                     | COMMUNICATION WITH DGRPS USES THE  | DGRP0620             |
|                     |  |                      |

C

CC

```
DGRP0630
DGRP0640
C
                                     FOLLOWING EPSJ = DSORT (UROUND),
C
                                     USED IN THE NUMERICAL JACOBIAN
С
                                      INCREMENTS.
                                                                         DGRP0650
C
                                                                          DGRP0660
                                  FIRST EXECUTABLE STATEMENT
C
                                                                         DGRP0670
      IF (NLC.EQ.-1) GO TO 45
                                                                          DGRP0680
                                  BANDED JACOBIAN CASE
C
                                                                          DGRP0690
      NB = NLC+NUC+1
                                                                          DGRP0700
      NWK = NB*N0+1
                                                                          DGRP0710
      IF (MITER.EQ.2) GO TO 15
                                                                          DGRP0720
                                  MITER = 1
C
                                                                          DGRP0730
      NLIM = NB*N0
                                                                          DGRP0740
      DO 5 I=1, NLIM
                                                                          DGRP0750
         PW(I) = 0.0D0
                                                                          DGRP0760
    5 CONTINUE
                                                                          DGRP0770
      CALL FCNJ (NC, T, Y, PW)
                                                                          DGRP0780
      DO 10 I=1, NLIM
                                                                          DGRP0790
         PW(I) = PW(I) *CON
                                                                          DGRP0800
   10 CONTINUE
                                                                          DGRP0810
      GO TO 35
                                                                          DGRP0820
                                 MITER = 2
C
                                                                          DGRP0830
   15 D = 0.0D0
                                                                          DGRP0840
      DO 20 I=1,NC
                                                                          DGRP0850
   20 D = D + SAVE2(I) **2
                                                                          DGRP0860
      R0 = DABS(H)*DSQRT(D)*1.0D+03*UROUND
                                                                          DGRP0870
      DO 30 J=1, NC
                                                                          DGRP0880
         YJ = Y(J,1)
                                                                          DGRP0890
         R = EPSJ*YMAX(J)
                                                                          DGRP0900
         R = DMAX1(R,R0)
                                                                          DGRP0910
         Y(J,1) = Y(J,1) + R
                                                                          DGRP0920
         D = CON/R
                                                                          DGRP0930
         CALL FCN(NC,T,Y,SAVE1)
                                                                          DGRP0940
      LIM1 = MAX0(1, J-NUC)
                                                                          DGRP0950
         LIM2 = MINO(N0, J+NLC)
                                                                          DGRP0960
      DO 25 I=LIM1,LIM2
                                                                          DGRP0970
                                                                         DGRP0980
             IJ = (J-I+NLC)*NO+I
             PW(IJ) = (SAVE1(I) - SAVE2(I)) *D
                                                                          DGRP0990
   25
         CONTINUE
                                                                          DGRP1000
                                                                         DGRP1010
         Y(J,1) = YJ
   30 CONTINUE
                                                                          DGRP1020
                               ADD IDENTITY MATRIX.
                                                                          DGRP1030
C
                                                                        DGRP1040
   35 DO 40 I=1, NC
         II = NLC*N0+I
                                                                          DGRP1050
         PW(II) = PW(II) + 1.0D0
                                                                          DGRP1060
   40 CONTINUE
                                                                          DGRP1070
C
                                    DO LU DECOMPOSITION ON P
                                                                          DGRP1080
C
                                                                          DGRP1090
      CALL LEQT1B (PW, NC, NLC, NUC, NO, EQUIL, 1, NO, 1, PW (NWK), IER)
                                                                          DGRP1100
      RETURN
                                                                          DGRP1110
                                                                          DGRP1120
                                    FULL JACOBIAN CASE
C
   45 IF (MITER.EQ.2) GO TO 55
                                                                          DGRP1130
                                    MITER = 1
C
                                                                          DGRP1140
      CALL FCNJ (NC, T, Y, PW)
                                                                          DGRP1150
      DO 50 I=1, NSQ
                                                                          DGRP1160
                                                                          DGRP1170
   50 \text{ PW}(I) = \text{PW}(I) * \text{CON}
      GO TO 75
                                                                          DGRP1180
                                  MITER = 2
                                                                          DGRP1190
   55 D = 0.0D0
                                                                          DGRP1200
      DO 60 I=1, NC
                                                                          DGRP1210
   60 D = D+SAVE2(I)**2
                                                                          DGRP1220
      R0 = DABS(H)*DSQRT(D)*1.0D+03*UROUND
                                                                          DGRP1230
                                                                          DGRP1240
       J1 = 0
```

|   | DO 7    | 0 J=1,NC   | DGRP1250 |
|---|---------|--|----------|
|   | Y       | J = Y(J, 1)  | DGRP1260 |
|   |         | = EPSJ*YMAX(J)   | DGRP1270 |
|   |         | = DMAX1(R,R0)  | DGRP1280 |
|   |         | (J,1) = Y(J,1) + R                                       | DGRP1290 |
|   |         | C = CON/R  | DGRP1300 |
|   |         | ·  |          |
|   |         | ALL FCN (NC, T, Y, SAVE1)                                | DGRP1310 |
|   |         | O 65 I=1,NC  | DGRP1320 |
|   |         | W(I+J1) = (SAVE1(I) - SAVE2(I)) *D                       | DGRP1330 |
|   | Y       | (J,1) = YJ   | DGRP1340 |
|   |         | 1 = J1 + N0  | DGRP1350 |
|   | 70 CONT | INUE   | DGRP1360 |
| C |         | ADD IDENTITY MATRIX.                                     | DGRP1370 |
| Ŭ | 75 J =  |  | DGRP1380 |
|   |         | 0 I=1,NC   | DGRP1390 |
|   |         | W(J) = PW(J) + 1.0D0                                     | DGRP1400 |
|   |         |  |          |
|   |         | I = J + (N0+1)   | DGRP1410 |
|   | 80 CONT |  | DGRP1420 |
| C |         | DO LU DECOMPOSITION ON P.                                | DGRP1430 |
| C |         |  | DGRP1440 |
|   | CALI    | LUDATF (PW, PW, NC, NO, 0, D1, D2, IPIV, EQUIL, WA, IER) | DGRP1450 |
|   | RETT    |  | DGRP1460 |
|   | END     |  | DGRP1470 |
|   | 2112    |  | 20111170 |

```
C
   IMSL ROUTINE NAME - DGRIN
                                                                      DGRI0010
C
                                                                      DGRI0020
                        -----DGRI0030
C-----
C
                                                                      DGRI0040
C
                       - IBM/DOUBLE
   COMPUTER
                                                                      DGRI0050
C
                                                                      DGRI0060
C
   LATEST REVISION
                     - JANUARY 1, 1978
                                                                      DGRI0070
C
                                                                      DGRI0080
C
   PURPOSE
                       - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR DGRI0090
C
                                                                      DGRI0100
C
   PRECISION/HARDWARE - SINGLE AND DOUBLE/H32
                                                                      DGRI0110
C
                       - SINGLE/H36,H48,H60
                                                                      DGRI0120
C
                                                                      DGRI0130
C
   REQD. IMSL ROUTINES - NONE REQUIRED
                                                                      DGRI0140
C
                                                                      DGRI0150
C
                      - INFORMATION ON SPECIAL NOTATION AND
   NOTATION
                                                                      DGRI0160
C
                          CONVENTIONS IS AVAILABLE IN THE MANUAL
                                                                     DGRI0170
C
                          INTRODUCTION OR THROUGH IMSL ROUTINE UHELP DGRI0180
C
                                                                      DGRI0190
C
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                                                                      DGRI0200
C
                                                                      DGRI0210
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C
   WARRANTY
                          APPLIED TO THIS CODE. NO OTHER WARRANTY,
                                                                   DGRI0230
C
                          EXPRESSED OR IMPLIED, IS APPLICABLE.
                                                                      DGRI0240
                                                                      DGRI0250
  -----DGRI0260
                                                                      DGRI0270
                        (TOUT, Y, NO, YO)
      SUBROUTINE DGRIN
                                                                      DGRI0280
                                 SPECIFICATIONS FOR ARGUMENTS
                                                                      DGRI0290
      INTEGER
                         N0
                                                                      DGRI0300
      DOUBLE PRECISION
                        TOUT, Y0 (N0), Y (N0, 1)
                                                                      DGRI0310
                                 SPECIFICATIONS FOR LOCAL VARIABLES
C
                                                                      DGRI0320
                       NC, MFC, KFLAG, I, L, J, JSTART, NSQ, NQUSED, NSTEP,
      INTEGER
                                                                      DGRI0330
                       NFE, NJE, NPW, NERROR, NSAVE1, NSAVE2, NEOUIL, NY,
                                                                      DGRI0340
     1
     2
                        IDUMMY (23)
                                                                      DGRI0350
      REAL
                        SDUMMY (4)
                                                                      DGRI0360
      DOUBLE PRECISION
                       T, H, HMIN, HMAX, EPSC, UROUND, EPSJ, HUSED, S, S1,
                                                                      DGRI0370
                        DUMMY (40)
                                                                      DGRI0380
      COMMON /GEAR/
                        T, H, HMIN, HMAX, EPSC, UROUND, EPSJ, HUSED, DUMMY,
                                                                      DGRI0390
                       SDUMMY, NC, MFC, KFLAG, JSTART, NSQ, NQUSED, NSTEP,
                                                                      DGRI0400
                       NFE, NJE, NPW, NERROR, NSAVE1, NSAVE2, NEQUIL, NY,
                                                                      DGRI0410
     3
                        IDUMMY
                                                                      DGRI0420
C
                                 FIRST EXECUTABLE STATEMENT
                                                                      DGRI0430
      DO 5 I = 1, NC
                                                                      DGRI0440
         YO(I) = Y(I,1)
                                                                      DGRI0450
    5 CONTINUE
                                                                      DGRI0460
C
                                 THIS SUBROUTINE COMPUTES INTERPOLATEDDGRI0470
C
                                   VALUES OF THE DEPENDENT VARIABLE DGRI0480
C
                                    Y AND STORES THEM IN YO. THE
                                                                      DGRI0490
C
                                    INTERPOLATION IS TO THE
                                                                      DGRI0500
C
                                                                      DGRI0510
                                    POINT T = TOUT, AND USES THE
C
                                   NORDSIECK HISTORY ARRAY Y, AS
                                                                      DGRI0520
C
                                   FOLLOWS..
                                                                      DGRI0530
C
                                               NQ
                                                                      DGRI0540
C
                                  Y0(I)
                                           = SUM Y(I,J+1)*S**J,
                                                                      DGRI0550
C
                                                                      DGRI0560
                                             J=0
C
                                WHERE S = -(T-TOUT)/H.
                                                                      DGRI0570
      L = JSTART + 1
                                                                      DGRI0580
      S = (TOUT - T)/H
                                                                      DGRI0590
      S1 = 1.0D0
                                                                      DGRI0600
      DO 15 J = 2, L
                                                                      DGRI0610
         S1 = S1*S
                                                                      DGRI0620
```

| DO 10 I = 1, NC              | DGRI0630 |
|------------------------------|----------|
| Y0 (I) = Y0 (I) + S1*Y(I, J) | DGRI0640 |
| 10 CONTINUE                  | DGR10650 |
| 15 CONTINUE                  | DGR10660 |
| RETURN                       | DGR10670 |
| END                          | DGR10680 |

| CCC         | IMSL ROUTINE     | NAME  | - LUDATF  | LUDA0010<br>LUDA0020 |
|-------------|------------------|-------|---|----------------------|
| C           |                  |       |   | LUDA0030             |
| C           | COMPUTER         |       | · · · · · · · · · · · · · · · · · · ·   | LUDA0050             |
| C           |                  |       |   | LUDA0060             |
| C           | LATEST REVIS     | ION   | ·   | LUDA0070             |
| C           | DINDOGR          |       |   | LUDA0080             |
| C           | PURPOSE          |       |   | LUDA0090<br>LUDA0100 |
| C           |                  |       |   | LUDA0110             |
| С           | USAGE            |       | - CALL LUDATF (A, LU, N, IA, IDGT, D1, D2, IPVT,  | LUDA0120             |
| С           |                  |       | EQUIL, WA, IER)   | LUDA0130             |
| C           | 2 D G ( D G ) TO | _     | THE WHENTY OF PINEWATON IS BY IT COMES THE  | LUDA0140             |
| C           | ARGUMENTS        | A     | - INPUT MATRIX OF DIMENSION N BY N CONTAINING THE MATRIX TO BE DECOMPOSED.                  | LUDA0150             |
| 00000000000 |                  | LU    | - REAL OUTPUT MATRIX OF DIMENSION N BY N  | LUDA0160<br>LUDA0170 |
| C           |                  | 10    | CONTAINING THE L-U DECOMPOSITION OF A   | LUDA0180             |
| C           |                  |       | ROWWISE PERMUTATION OF THE INPUT MATRIX.  | LUDA0190             |
| C           |                  |       | FOR A DESCRIPTION OF THE FORMAT OF LU, SEE  | LUDA0200             |
| С           |                  |       | EXAMPLE.  | LUDA0210             |
| C           |                  | N     |   | LUDA0220             |
| C           |                  | T.3   | MATRIX A.   | LUDA0230             |
| C           |                  | IA    | - INPUT SCALAR CONTAINING THE ROW DIMENSION OF<br>MATRICES A AND LU EXACTLY AS SPECIFIED IN | LUDA0240<br>LUDA0250 |
| 2           |                  |       | THE CALLING PROGRAM.  | LUDA0260             |
| Č           |                  | IDGT  |   | LUDA0270             |
| С           |                  |       | IF IDGT IS GREATER THAN ZERO, THE NON-ZERO  | LUDA0280             |
| С           |                  |       | ELEMENTS OF A ARE ASSUMED TO BE CORRECT TO  | LUDA0290             |
| C           |                  |       | IDGT DECIMAL PLACES. LUDATF PERFORMS AN   | LUDA0300             |
| C           |                  |       | ACCURACY TEST TO DETERMINE IF THE COMPUTED  | LUDA0310             |
| 00000000000 |                  |       | DECOMPOSITION IS THE EXACT DECOMPOSITION OF A MATRIX WHICH DIFFERS FROM THE GIVEN           | LUDA0320<br>LUDA0330 |
| 2           |                  |       | ONE BY LESS THAN ITS UNCERTAINTY.   | LUDA0340             |
| C           |                  |       | IF IDGT IS EQUAL TO ZERO, THE ACCURACY TEST   | LUDA0350             |
| Ċ           |                  |       | IS BYPASSED.  | LUDA0360             |
| С           |                  | D1    | - OUTPUT SCALAR CONTAINING ONE OF THE TWO   | LUDA0370             |
| C           |                  |       | COMPONENTS OF THE DETERMINANT. SEE  | LUDA0380             |
| C           |                  | D2    | DESCRIPTION OF PARAMETER D2, BELOW.   | LUDA0390<br>LUDA0400 |
| 0 0 0       |                  | D2    | - OUTPUT SCALAR CONTAINING ONE OF THE TWO COMPONENTS OF THE DETERMINANT. THE                | LUDA0410             |
| C           |                  |       | DETERMINANT MAY BE EVALUATED AS (D1) (2**D2)  |                      |
| Č           |                  | IPVT  | - OUTPUT VECTOR OF LENGTH N CONTAINING THE  | LUDA0430             |
| С           |                  |       | PERMUTATION INDICES. SEE DOCUMENT   | LUDA0440             |
| C           |                  |       | (ALGORITHM).  | LUDA0450             |
| C           |                  | EQUIL | - OUTPUT VECTOR OF LENGTH N CONTAINING  | LUDA0460             |
| C           |                  |       |   | LUDA0470<br>LUDA0480 |
| C           |                  |       | THE LARGEST (IN ABSOLUTE VALUE) ELEMENT IN EACH ROW.  | LUDA0490             |
| C           |                  | AW    | - ACCURACY TEST PARAMETER, OUTPUT ONLY IF   | LUDA0500             |
| Ċ           |                  |       | IDGT IS GREATER THAN ZERO.  | LUDA0510             |
| C           |                  |       | SEE ELEMENT DOCUMENTATION FOR DETAILS.  | LUDA0520             |
| C           |                  | IER   | - ERROR PARAMETER. (OUTPUT)   | LUDA0530             |
| C           |                  |       | TERMINAL ERROR  | LUDA0540             |
| C           |                  |       |   | LUDA0550<br>LUDA0560 |
| C           |                  |       | CHAPTER L PRELUDE).   | LUDA0570             |
| C           |                  |       | WARNING ERROR   | LUDA0580             |
| С           |                  |       | IER = 34 INDICATES THAT THE ACCURACY TEST   | LUDA0590             |
| C           |                  |       | FAILED. THE COMPUTED SOLUTION MAY BE IN   |                      |
| C           |                  |       |   | LUDA0610             |
| С           |                  |       | BY THE UNCERTAINTY OF THE DATA. THIS  | LUDA0620             |

```
WARNING CAN BE PRODUCED ONLY IF IDGT IS
                                                                          LUDA0630
                                                                          LUDA0640
GREATER THAN O ON INPUT. SEE CHAPTER L
                              PRELUDE FOR FURTHER DISCUSSION.
                                                                          LUDA0650
                                                                          LUDA0660
    PRECISION/HARDWARE
                        - SINGLE AND DOUBLE/H32
                                                                          LUDA0670
                        - SINGLE/H36, H48, H60
                                                                          LUDA0680
                                                                          LUDA0690
    REOD. IMSL ROUTINES - UERTST, UGETIO
                                                                          LUDA0700
                                                                          LUDA0710
                        - INFORMATION ON SPECIAL NOTATION AND
   NOTATION
                                                                          LUDA0720
                            CONVENTIONS IS AVAILABLE IN THE MANUAL
                                                                          LUDA0730
                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
                                                                          LUDA0740
                                                                          LUDA0750
                A TEST FOR SINGULARITY IS MADE AT TWO LEVELS:
    REMARKS
                                                                          LUDA0760
                1. A ROW OF THE ORIGINAL MATRIX A IS NULL.
                                                                          LUDA0770
                2. A COLUMN BECOMES NULL IN THE FACTORIZATION PROCESS.LUDA0780
                                                                          LUDA0790
    COPYRIGHT
                        - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.
                                                                          LUDA0800
                                                                          LUDA0810
                        - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN LUDA0820
    WARRANTY
                            APPLIED TO THIS CODE. NO OTHER WARRANTY,
                                                                          LUDA0830
                            EXPRESSED OR IMPLIED, IS APPLICABLE.
                                                                          LUDA0840
C
                                                                          LUDA0850
C-
                                                                          -LUDA0860
C
                                                                          LUDA0870
      SUBROUTINE LUDATF (A, LU, N, IA, IDGT, D1, D2, IPVT, EQUIL, WA, IER)
                                                                          LUDA0880
C
                                                                          LUDA0890
      DIMENSION
                         A(IA,1),LU(IA,1),IPVT(1),EQUIL(1)
                                                                          LUDA0900
      DOUBLE PRECISION A, LU, D1, D2, EQUIL, WA, ZERO, ONE, FOUR, SIXTN, SIXTH, LUDA0910
                         RN, WREL, BIGA, BIG, P, SUM, AI, WI, T, TEST, Q
                                                                          LUDA0920
      DATA
                         ZERO, ONE, FOUR, SIXTN, SIXTH/0.D0, 1.D0, 4.D0,
                                                                          LUDA0930
                         16.D0,.0625D0/
                                                                          LUDA0940
C
                                   FIRST EXECUTABLE STATEMENT
                                                                          LUDA0950
C
                                   INITIALIZATION
                                                                          LUDA0960
      IER = 0
                                                                          LUDA0970
      RN = N
                                                                          LUDA0980
      WREL = ZERO
                                                                          LUDA0990
      D1 = ONE
                                                                          LUDA1000
      D2 = ZERO
                                                                          LUDA1010
      BIGA = ZERO
                                                                          LUDA1020
      DO 10 I=1, N
                                                                          LUDA1030
         BIG = ZERO
                                                                          LUDA1040
         DO 5 J=1, N
                                                                          LUDA1050
            P = A(I,J)
                                                                          LUDA1060
            LU(I,J) = P
                                                                          LUDA1070
            P = DABS(P)
                                                                          LUDA1080
            IF (P .GT. BIG) BIG = P
                                                                          LUDA1090
    5
         CONTINUE
                                                                          LUDA1100
         IF (BIG .GT. BIGA) BIGA = BIG
                                                                          LUDA1110
         IF (BIG .EQ. ZERO) GO TO 110
                                                                          LUDA1120
         EQUIL(I) = ONE/BIG
                                                                          LUDA1130
   10 CONTINUE
                                                                           LUDA1140
      DO 105 J=1, N
                                                                           LUDA1150
         JM1 = J-1
                                                                           LUDA1160
         IF (JM1 .LT. 1) GO TO 40
                                                                           LUDA1170
                                    COMPUTE U(I,J), I=1,...,J-1
                                                                           LUDA1180
         DO 35 I=1, JM1
                                                                           LUDA1190
             SUM = LU(I,J)
                                                                           LUDA1200
             IM1 = I-1
                                                                           LUDA1210
             IF (IDGT .EQ. 0) GO TO 25
                                                                           LUDA1220
C
                                                                           LUDA1230
                                    WITH ACCURACY TEST
            AI = DABS(SUM)
                                                                          LUDA1240
```

```
WI = ZERO
                                                                           LUDA1250
            IF (IM1 .LT. 1) GO TO 20
                                                                           LUDA1260
            DO 15 K=1, IM1
                                                                           LUDA1270
                T = LU(I,K) *LU(K,J)
                                                                           LUDA1280
                SUM = SUM-T
                                                                           LUDA1290
                WI = WI + DABS(T)
                                                                           LUDA1300
            CONTINUE
   15
                                                                           LUDA1310
            LU(I,J) = SUM
                                                                           LUDA1320
   20
            WI = WI + DABS (SUM)
                                                                           LUDA1330
            IF (AI .EQ. ZERO) AI = BIGA
                                                                           LUDA1340
            TEST = WI/AI
                                                                           LUDA1350
             IF (TEST .GT. WREL) WREL = TEST
                                                                           LUDA1360
             GO TO 35
                                                                           LUDA1370
C
                                    WITHOUT ACCURACY
                                                                           LUDA1380
            IF (IM1 .LT. 1) GO TO 35
   25
                                                                           LUDA1390
             DO 30 K=1, IM1
                                                                           LUDA1400
                SUM = SUM - LU(I,K) * LU(K,J)
                                                                           LUDA1410
   30
            CONTINUE
                                                                           LUDA1420
             LU(I,J) = SUM
                                                                           LUDA1430
   35
         CONTINUE
                                                                           LUDA1440
   40
         P = ZERO
                                                                           LUDA1450
C
                                   COMPUTE U(J,J) AND L(I,J), I=J+1,...,LUDA1460
         DO 70 I=J, N
                                                                           LUDA1470
             SUM = LU(I,J)
                                                                           LUDA1480
             IF (IDGT .EQ. 0) GO TO 55
                                                                           LUDA1490
C
                                    WITH ACCURACY TEST
                                                                           LUDA1500
             AI = DABS(SUM)
                                                                           LUDA1510
             WI = ZERO
                                                                           LUDA1520
             IF (JM1 .LT. 1) GO TO 50
                                                                           LUDA1530
             DO 45 K=1,JM1
                                                                           LUDA1540
                T = LU(I,K) *LU(K,J)
                                                                           LUDA1550
                SUM = SUM-T
                                                                           LUDA1560
                WI = WI + DABS(T)
                                                                           LUDA1570
   45
             CONTINUE
                                                                           LUDA1580
             LU(I,J) = SUM
                                                                           LUDA1590
            WI = WI + DABS (SUM)
   50
                                                                           LUDA1600
             IF (AI .EQ. ZERO) AI = BIGA
                                                                           LUDA1610
             TEST = WI/AI
                                                                           LUDA1620
             IF (TEST .GT. WREL) WREL = TEST
                                                                           LUDA1630
             GO TO 65
                                                                           LUDA1640
C
                                    WITHOUT ACCURACY TEST
                                                                           LUDA1650
   55
            IF (JM1 .LT. 1) GO TO 65
                                                                           LUDA1660
             DO 60 K=1, JM1
                                                                           LUDA1670
                SUM = SUM - LU(I,K) * LU(K,J)
                                                                           LUDA1680
             CONTINUE
   60
                                                                           LUDA1690
             LU(I,J) = SUM
                                                                           LUDA1700
             Q = EQUIL(I) *DABS(SUM)
                                                                           LUDA1710
   65
             IF (P .GE. Q) GO TO 70
                                                                            LUDA1720
             P = Q
                                                                            LUDA1730
             IMAX = I
                                                                            LUDA1740
   70
         CONTINUE
                                                                           LUDA1750
                                                                           LUDA1760
C
                                    TEST FOR ALGORITHMIC SINGULARITY
          IF (RN+P .EQ. RN) GO TO 110
                                                                           LUDA1770
                                                                           LUDA1780
          IF (J .EQ. IMAX) GO TO 80
                                                                            LUDA1790
C
                                    INTERCHANGE ROWS J AND IMAX
          D1 = -D1
                                                                            LUDA1800
          DO 75 K=1, N
                                                                            LUDA1810
             P = LU(IMAX, K)
                                                                            LUDA1820
             LU(IMAX,K) = LU(J,K)
                                                                            LUDA1830
             LU(J,K) = P
                                                                            LUDA1840
   75
          CONTINUE
                                                                            LUDA1850
          EQUIL(IMAX) = EQUIL(J)
                                                                            LUDA1860
```

| 80     | IPVT(J) = IMAX $D1 = D1*LU(J,J)$          | LUDA1870<br>LUDA1880 |
|--------|---|----------------------|
| 85     | IF (DABS(D1) .LE. ONE) GO TO 90           | LUDA1890             |
| 83     | D1 = D1*SIXTH                             | LUDA1900             |
|        | D2 = D2+FOUR                              | LUDA1910             |
|        | GO TO 85                                  | LUDA1920             |
| 90     | IF (DABS(D1) .GE. SIXTH) GO TO 95         | LUDA1930             |
| 70     | D1 = D1*SIXTN                             | LUDA1940             |
|        | D2 = D2-FOUR                              | LUDA1950             |
|        | GO TO 90                                  | LUDA1960             |
| 95     | CONTINUE                                  | LUDA1970             |
|        | JP1 = J+1                                 | LUDA1980             |
|        | IF (JP1 .GT. N) GO TO 105                 | LUDA1990             |
| C      | DIVIDE BY PIVOT ELEMENT U(J,J)            | LUDA2000             |
|        | P = LU(J,J)                               | LUDA2010             |
|        | DO 100 I=JP1,N                            | LUDA2020             |
|        | LU(I,J) = LU(I,J)/P                       | LUDA2030             |
| 100    | CONTINUE                                  | LUDA2040             |
|        | CONTINUE                                  | LUDA2050             |
| C      | PERFORM ACCURACY TEST                     | LUDA2060             |
|        | IF (IDGT .EQ. 0) GO TO 9005               | LUDA2070             |
|        | P = 3*N+3                                 | LUDA2080             |
|        | WA = P*WREL                               | LUDA2090             |
|        | IF (WA+10.D0**(-IDGT) .NE. WA) GO TO 9005 | LUDA2100             |
|        | IER = 34                                  | LUDA2110             |
| _      | GO TO 9000                                | LUDA2120             |
| C 110  | ALGORITHMIC SINGULARITY                   | LUDA2130             |
| 110    | IER = 129<br>D1 = ZERO                    | LUDA2140<br>LUDA2150 |
|        | D1 = ZERO<br>D2 = ZERO                    | LUDA2150             |
| 9000   | CONTINUE                                  | LUDA2180<br>LUDA2170 |
| C 2000 | PRINT ERROR                               | LUDA2170             |
| _      | CALL UERTST (IER, 6HLUDATF)               | LUDA2180             |
| 9005   | RETURN                                    | LUDA2200             |
| 7003   | END                                       | LUDA2210             |
|        |   |                      |

.

```
IMSL ROUTINE NAME - LUELMF
С
                                                                      LUEF0010
C
                                                                      LUEF0020
   ------LUEF0030
C-
C
                                                                      LUEF0040
C
                      - IBM/DOUBLE
   COMPUTER
                                                                      LUEF0050
C
                                                                      LUEF0060
C
   LATEST REVISION - JANUARY 1, 1978
                                                                      LUEF0070
C
                                                                      LUEF0080
C
                       - ELIMINATION PART OF SOLUTION OF AX=B
   PURPOSE
                                                                      LUEF0090
Ĉ
                         (FULL STORAGE MODE)
                                                                      LUEF0100
Č
                                                                      LUEF0110
00000000
   USAGE
                       - CALL LUELMF (A,B,IPVT,N,IA,X)
                                                                      LUEF0120
                                                                      LUEF0130
                       - A = LU (THE RESULT COMPUTED IN THE IMSL
ROUTINE LUDATF) WHERE L IS A LOWER
                                                                    LUEF0140
   ARGUMENTS A
                                                                      LUEF0150
                          TRIANGULAR MATRIX WITH ONES ON THE MAIN
                                                                      LUEF0160
                          DIAGONAL. U IS UPPER TRIANGULAR. L AND U
                                                                      LUEF0170
                          ARE STORED AS A SINGLE MATRIX A AND THE
                                                                      LUEF0180
                          UNIT DIAGONAL OF L IS NOT STORED. (INPUT)
                                                                      LUEF0190
C
                       - B IS A VECTOR OF LENGTH N ON THE RIGHT HAND
                                                                      LUEF0200
                           SIDE OF THE EQUATION AX=B. (INPUT)
                                                                      LUEF0210
C
                IPVT
                       - THE PERMUTATION MATRIX RETURNED FROM THE
                                                                      LUEF0220
C
                          IMSL ROUTINE LUDATF, STORED AS AN N LENGTH LUEF0230
                           VECTOR. (INPUT)
                                                                      LUEF0240
C
                       - ORDER OF A AND NUMBER OF ROWS IN B. (INPUT)
                                                                    LUEF0250
                       - ROW DIMENSION OF A EXACTLY AS SPECIFIED IN
С
                TA
                                                                      LUEF0260
C
                           THE DIMENSION STATEMENT IN THE CALLING
                                                                      LUEF0270
                       PROGRAM. (INPUT)
- THE RESULT X. (OUTPUT)
С
                                                                      LUEF0280
C
                                                                      LUEF0290
C
                                                                      LUEF0300
C
    PRECISION/HARDWARE - SINGLE AND DOUBLE/H32
                                                                      LUEF0310
C
                       - SINGLE/H36, H48, H60
                                                                      LUEF0320
C
                                                                      LUEF0330
C
    REQD. IMSL ROUTINES - NONE REQUIRED
                                                                      LUEF0340
C
                                                                      LUEF0350
                       - INFORMATION ON SPECIAL NOTATION AND LUEF0360 CONVENTIONS IS AVAILABLE IN THE MANUAL LUEF0370
С
    NOTATION
С
C
                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP LUEF0380
C
                                                                      LUEF0390
C
                      - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.
    COPYRIGHT
                                                                      LUEF0400
С
                                                                      LUEF0410
C
    WARRANTY - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN LUEF0420
                         APPLIED TO THIS CODE. NO OTHER WARRANTY, LUEF0430
C
C
                          EXPRESSED OR IMPLIED, IS APPLICABLE.
                                                                      LUEF0440
C
                                                                      LUEF0450
     ------LUEF0460
C
C
                                                                      LUEF0470
      SUBROUTINE LUELMF (A,B,IPVT,N,IA,X)
                                                                      LUEF0480
                                                                      LUEF0490
     DIMENSION
                        A(IA,1),B(1),IPVT(1),X(1)
                                                                      LUEF0500
      DOUBLE PRECISION
                       A,B,X,SUM
                                                                      LUEF0510
C
                                 FIRST EXECUTABLE STATEMENT
                                                                      LUEF0520
C
                                  SOLVE LY = B FOR Y
                                                                      LUEF0530
     DO 5 I=1, N
                                                                      LUEF0540
    5 X(I) = B(I)
                                                                      LUEF0550
      IW = 0
                                                                      LUEF0560
      DO 20 I=1, N
                                                                      LUEF0570
         IP = IPVT(I)
                                                                       LUEF0580
         SUM = X(IP)
                                                                       LUEF0590
         X(IP) = X(I)
                                                                       LUEF0600
         IF (IW .EQ. 0) GO TO 15
                                                                       LUEF0610
         IM1 = I-1
                                                                       LUEF0620
```

```
DO 10 J=IW, IM1
                                                                      LUEF0630
        SUM = SUM - A(I,J) *X(J)
                                                                      LUEF0640
      CONTINUE
                                                                      LUEF0650
      GO TO 20
                                                                      LUEF0660
    IF (SUM .NE. 0.D0) IW = I
                                                                      LUEF0670
20 X(I) = SUM
                                                                      LUEF0680
                               SOLVE UX = Y FOR X
                                                                      LUEF0690
   DO 30 IB=1,N
                                                                      LUEF0700
      I = N+1-IB
                                                                      LUEF0710
      IP1 = I+1
                                                                      LUEF0720
      SUM = X(I)
                                                                      LUEF0730
      IF (IP1 .GT. N) GO TO 30
                                                                      LUEF0740
      DO 25 J=IP1, N
                                                                      LUEF0750
        SUM = SUM - A(I, J) *X(J)
                                                                      LUEF0760
25 CONTINUE
                                                                      LUEF0770
30 \times (I) = SUM/A(I,I)
                                                                      LUEF0780
  RETURN
                                                                      LUEF0790
   END
                                                                      LUEF0800
```

| ~      | TMCI DOUTENE | NTA ME | I DOTED  | T E 1 B 0 0 1 0      |
|--------|--------------|--------|--|----------------------|
| C      | IMSL ROUTINE | NAME   | - LEQT1B   | LE1B0010             |
| C      |              |        |  | LE1B0020             |
| C      |              |        |  | LE1B0040             |
| C      | COMPUTER     |        | - IBM/DOUBLE   | LE1B0050             |
| C      |              |        |  | LE1B0060             |
| C      | LATEST REVIS | ION    | - JANUARY 1, 1978  | LE1B0070             |
| С      |              |        |  | LE1B0080             |
| С      | PURPOSE      |        |  | LE1B0090             |
| C      |              |        |  | LE1B0100             |
| C      |              |        |  | LE1B0110             |
| C      | USAGE        |        |  |                      |
| C      |              |        |  | LE1B0130<br>LE1B0140 |
| C<br>C | ADCHMENTS    | Δ      |  |                      |
| C      | ARGUMENTS    | A      | - INPUT/OUTPUT MATRIX OF DIMENSION N BY (NUC+NLC+1). SEE PARAMETER IJOB.               | LE1B0150             |
| C      |              | N      | - ORDER OF MATRIX A AND THE NUMBER OF ROWS IN  | LE1B0170             |
| ď      |              |        |  | LE1B0180             |
| C<br>C |              | NLC    |  | LE1B0190             |
| С      |              |        | (INPUT)  | LE1B0200             |
| C      |              | NUC    | - NUMBER OF UPPER CODIAGONALS IN MATRIX A.   | LE1B0210             |
| C      |              |        | (INPUT)  | LE1B0220             |
| С      |              | IA     |  | LE1B0230             |
| С      |              |        | SPECIFIED IN THE DIMENSION STATEMENT IN THE  |                      |
| C      |              |        |  | LE1B0250             |
| C      |              | В      | - INPUT/OUTPUT MATRIX OF DIMENSION N BY M.   |                      |
| C      |              |        | ON INPUT, B CONTAINS THE M RIGHT-HAND SIDES  |                      |
| C      |              |        | OF THE EQUATION AX = B. ON OUTPUT, THE   |                      |
| C      |              |        | SOLUTION MATRIX X REPLACES B. IF IJOB = 1,<br>B IS NOT USED.                           | LE1B0290             |
| C      |              | М      | - NUMBER OF RIGHT HAND SIDES (COLUMNS IN B).   |                      |
| C      |              | **     |  | LE1B0320             |
| C      |              | IB     | · · · · · · · · · · · · · · · · · · ·  | LE1B0330             |
| C      |              |        | SPECIFIED IN THE DIMENSION STATEMENT IN THE  |                      |
| Ċ      |              |        | CALLING PROGRAM. (INPUT)   | LE1B0350             |
| C      |              | IJOB   | - INPUT OPTION PARAMETER. IJOB = I IMPLIES WHEN  | LE1B0360             |
| C      |              |        | I = 0, FACTOR THE MATRIX A AND SOLVE THE   |                      |
| 0 0    |              |        | EQUATION AX = B. ON INPUT, A CONTAINS THE  |                      |
| C      |              |        | COEFFICIENT MATRIX OF THE EQUATION AX = B  |                      |
| C      |              |        | WHERE A IS ASSUMED TO BE AN N BY N BAND  |                      |
| C      |              |        | MATRIX. A IS STORED IN BAND STORAGE MODE   | LE1B0410             |
| C      |              |        | AND THEREFORE HAS DIMENSION N BY (NLC+NUC+1). ON OUTPUT, A IS REPLACED                 | LE1B0420             |
| С      |              |        |  |                      |
| C      |              |        | BY THE U MATRIX OF THE L-U DECOMPOSITION OF A ROWWISE PERMUTATION OF MATRIX A. U       | LE1B0440<br>LE1B0450 |
| C<br>C |              |        | IS STORED IN BAND STORAGE MODE.  | LE1B0450             |
| C      |              |        | I = 1, FACTOR THE MATRIX A. A CONTAINS THE   | LE1B0470             |
| C      |              |        | SAME INPUT/OUTPUT INFORMATION AS IF  | LE1B0480             |
| Ċ      |              |        | IJOB = 0.  | LE1B0490             |
| C      |              |        | I = 2, SOLVE THE EQUATION AX = B. THIS   | LE1B0500             |
| C      |              |        | OPTION IMPLIES THAT LEQT1B HAS ALREADY   | LE1B0510             |
| C      |              |        | BEEN CALLED USING IJOB = 0 OR 1 SO THAT  | LE1B0520             |
| С      |              |        | THE MATRIX A HAS ALREADY BEEN FACTORED.  | LE1B0530             |
| C      |              |        | IN THIS CASE, OUTPUT MATRICES A AND XL   | LE1B0540             |
| C      |              |        | MUST HAVE BEEN SAVED FOR REUSE IN THE  | LE1B0550             |
| C      |              | VI     | CALL TO LEQT1B.  | LE1B0560             |
| C      |              | XL     | · · · · · · · · · · · · · · · · · · ·  | LE1B0570             |
| C      |              |        | NLC*N LOCATIONS OF XL CONTAIN COMPONENTS OF THE L MATRIX OF THE L-U DECOMPOSITION OF A |                      |
| C      |              |        | ROWWISE PERMUTATION OF A. THE LAST N   | LE1B0590             |
| C      |              |        | LOCATIONS CONTAIN THE PIVOT INDICES.   | LE1B0610             |
| C      |              | IER    | - ERROR PARAMETER. (OUTPUT)  | LE1B0620             |
|        |              |        | ,,   |                      |

```
TERMINAL ERROR
                                                                      LE1B0630
                          IER = 129 INDICATES THAT MATRIX A IS
                            ALGORITHMICALLY SINGULAR. (SEE THE
                             CHAPTER L PRELUDE).
   PRECISION/HARDWARE - SINGLE AND DOUBLE/H32
                                                                      LE1B0680
                       - SINGLE/H36.H48.H60
   REOD. IMSL ROUTINES - UERTST, UGETIO
                                                                      LE1B0710
   NOTATION
                       - INFORMATION ON SPECIAL NOTATION AND
                          CONVENTIONS IS AVAILABLE IN THE MANUAL
                          INTRODUCTION OR THROUGH IMSL ROUTINE UHELP LE1B0750
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   WARRANTY
                      - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN LE1B0790
                          APPLIED TO THIS CODE. NO OTHER WARRANTY,
                          EXPRESSED OR IMPLIED, IS APPLICABLE.
C-
         --------------LE1B0830
      SUBROUTINE LEQT1B (A,N,NLC,NUC,IA,B,M,IB,IJOB,XL,IER)
      DIMENSION
                        A(IA,1), XL(N,1), B(IB,1)
      DOUBLE PRECISION
                       A, XL, B, P, Q, ZERO, ONE, RN
                                                                      LE1B0880
                        ZERO/0.D0/,ONE/1.0D0/
      DATA
                                 FIRST EXECUTABLE STATEMENT
                                                                      LE1B0900
      IER = 0
                                                                      LE1B0910
      JBEG = NLC+1
                                                                      LE1B0920
      NLC1 = JBEG
                                                                      LE1B0930
      IF (IJOB .EQ. 2) GO TO 80
                                                                      LE1B0940
      RN = N
                                                                      LE1B0950
                                  RESTRUCTURE THE MATRIX
                                                                      LE1B0960
                                  FIND RECIPROCAL OF THE LARGEST
                                                                      LE1B0970
                                 ABSOLUTE VALUE IN ROW I
                                                                      LE1B0980
      I = 1
                                                                      LE1B0990
      NC = JBEG+NUC
                                                                      LE1B1000
      NN = NC
                                                                      LE1B1010
      JEND = NC
                                                                      LE1B1020
      IF (N .EQ. 1 .OR. NLC .EQ. 0) GO TO 25
                                                                      LE1B1030
    5 K = 1
                                                                      LE1B1040
      P = ZERO
                                                                      LE1B1050
      DO 10 J = JBEG, JEND
                                                                      LE1B1060
        A(I,K) = A(I,J)
                                                                      LE1B1070
         O = DABS(A(I,K))
                                                                      LE1B1080
         IF (Q .GT. P) P = Q
                                                                      LE1B1090
         K = K+1
                                                                       LE1B1100
   10 CONTINUE
                                                                       LE1B1110
      IF (P .EQ. ZERO) GO TO 135
                                                                       LE1B1120
      XL(I,NLC1) = ONE/P
                                                                       LE1B1130
      IF (K .GT. NC) GO TO 20
                                                                       LE1B1140
      DO 15 J = K,NC
                                                                       LE1B1150
        A(I,J) = ZERO
                                                                       LE1B1160
   15 CONTINUE
                                                                       LE1B1170
   20 I = I+1
                                                                       LE1B1180
      JBEG = JBEG-1
                                                                       LE1B1190
      IF (JEND-JBEG . EQ. N) JEND = JEND-1
                                                                       LE1B1200
      IF (I .LE. NLC) GO TO 5
                                                                       LE1B1210
      JBEG = I
                                                                       LE1B1220
      NN = JEND
                                                                       LE1B1230
   25 \text{ JEND} = \text{N-NUC}
                                                                       LE1B1240
```

C C

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C

C

C

C

C

C

```
DO 40 I = JBEG, N
                                                                           LE1B1250
         P = ZERO
                                                                           LE1B1260
         DO 30 J = 1,NN
                                                                           LE1B1270
            O = DABS(A(I,J))
                                                                           LE1B1280
            IF (Q .GT. P) P = Q
                                                                           LE1B1290
         CONTINUE
   30
                                                                           LE1B1300
         IF (P .EQ. ZERO) GO TO 135
                                                                           LE1B1310
         XL(I,NLC1) = ONE/P
                                                                           LE1B1320
         IF (I .EQ. JEND) GO TO 37
                                                                           LE1B1330
         IF (I .LT. JEND) GO TO 40
                                                                           LE1B1340
         K = NN+1
                                                                           LE1B1350
         DO 35 J = K,NC
                                                                           LE1B1360
            A(I,J) = ZERO
                                                                           LE1B1370
         CONTINUE
   35
                                                                           LE1B1380
         NN = NN-1
   37
                                                                           LE1B1390
   40 CONTINUE
                                                                           LE1B1400
      L = NLC
                                                                           LE1B1410
C
                                    L-U DECOMPOSITION
                                                                           LE1B1420
      DO 75 K = 1, N
                                                                           LE1B1430
         P = DABS(A(K,1))*XL(K,NLC1)
                                                                           LE1B1440
         I = K
                                                                           LE1B1450
         IF (L . LT . N) L = L+1
                                                                           LE1B1460
         K1 = K+1
                                                                           LE1B1470
         IF (K1 .GT. L) GO TO 50
                                                                           LE1B1480
         DO 45 J = K1, L
                                                                           LE1B1490
             Q = DABS(A(J,1))*XL(J,NLC1)
                                                                           LE1B1500
                                                                           LE1B1510
             IF (Q .LE. P) GO TO 45
             P = Q
                                                                           LE1B1520
             I = J
                                                                           LE1B1530
   45
         CONTINUE
                                                                           LE1B1540
   50
         XL(I,NLC1) = XL(K,NLC1)
                                                                           LE1B1550
         XL(K,NLC1) = I
                                                                           LE1B1560
C
                                    SINGULARITY FOUND
                                                                           LE1B1570
         Q = RN+P
                                                                           LE1B1580
         IF (Q .EQ. RN) GO TO 135
                                                                           LE1B1590
C
                                    INTERCHANGE ROWS I AND K
                                                                           LE1B1600
                                                                           LE1B1610
         IF (K .EQ. I) GO TO 60
                                                                           LE1B1620
         DO 55 J = 1, NC
             P = A(K,J)
                                                                           LE1B1630
             A(K,J) = A(I,J)
                                                                           LE1B1640
             A(I,J) = P
                                                                           LE1B1650
         CONTINUE
                                                                           LE1B1660
   55
         IF (K1 .GT. L) GO TO 75
                                                                           LE1B1670
   60
         DO 70 I = K1,L
                                                                           LE1B1680
             P = A(I,1)/A(K,1)
                                                                           LE1B1690
             IK = I - K
                                                                           LE1B1700
             XL(K1,IK) = P
                                                                           LE1B1710
             DO 65 J = 2,NC
                                                                           LE1B1720
                A(I,J-1) = A(I,J) - P*A(K,J)
                                                                           LE1B1730
   65
         CONTINUE
                                                                           LE1B1740
         A(I,NC) = ZERO
                                                                           LE1B1750
   70
         CONTINUE
                                                                           LE1B1760
   75 CONTINUE
                                                                           LE1B1770
      IF (IJOB .EQ. 1) GO TO 9005
                                                                           LE1B1780
C
                                    FORWARD SUBSTITUTION
                                                                           LE1B1790
   80 L = NLC
                                                                           LE1B1800
      DO 105 K = 1.N
                                                                           LE1B1810
          I = XL(K, NLC1)
                                                                           LE1B1820
          IF (I .EQ. K) GO TO 90
                                                                           LE1B1830
         DO 85 J = 1.M
                                                                           LE1B1840
             P = B(K, J)
                                                                           LE1B1850
             B(K,J) = B(I,J)
                                                                           LE1B1860
```

```
LE1B1870
            B(I,J) = P
                                                                         LE1B1880
         CONTINUE
   85
                                                                         LE1B1890
         IF (L .LT. N) L = L+1
   90
                                                                         LE1B1900
         K1 = K+1
         IF (K1 .GT. L) GO TO 105
                                                                         LE1B1910
         DO 100 I = K1,L
                                                                         LE1B1920
                                                                         LE1B1930
            IK = I - K
            P = XL(K1, IK)
                                                                         LE1B1940
                                                                         LE1B1950
            DO 95 J = 1, M
            B(I,J) = B(I,J) - P*B(K,J)
                                                                         LE1B1960
            CONTINUE
                                                                         LE1B1970
                                                                         LE1B1980
         CONTINUE
  100
                                                                         LE1B1990
  105 CONTINUE
                                  BACKWARD SUBSTITUTION
                                                                         LE1B2000
C
                                                                         LE1B2010
      JBEG = NUC+NLC
      DO 125 J = 1, M
                                                                         LE1B2020
                                                                         LE1B2030
         L = 1
         K1 = N+1
                                                                         LE1B2040
         DO 120 I = 1.N
                                                                         LE1B2050
                                                                         LE1B2060
            K = K1 - I
                                                                         LE1B2070
            P = B(K,J)
            IF (L .EQ. 1) GO TO 115
                                                                         LE1B2080
            DO 110 KK = 2,L
                                                                         LE1B2090
               IK = KK+K
                                                                         LE1B2100
               P = P-A(K,KK)*B(IK-1,J)
                                                                         LE1B2110
                                                                         LE1B2120
  110
            CONTINUE
                                                                         LE1B2130
            B(K,J) = P/A(K,1)
           IF (L .LE. JBEG) L = L+1
                                                                         LE1B2140
         CONTINUE
                                                                         LE1B2150
  120
                                                                         LE1B2160
  125 CONTINUE
      GO TO 9005
                                                                         LE1B2170
                                                                         LE1B2180
  135 IER = 129
 9000 CONTINUE
                                                                         LE1B2190
      CALL UERTST (IER, 6HLEQT1B)
                                                                         LE1B2200
 9005 RETURN
                                                                         LE1B2210
      END
                                                                         LE1B2220
```

| С      | IMSL ROUTINE | NAME -       | UERTST  | UERT0010             |
|--------|--------------|--------------|---|----------------------|
| С      |              |              |   | UERT0020             |
| C      |              |              |   | -UERT0030            |
| C      |              |              |   | UERT0040             |
| C      | COMPUTER     | _            | TDM /CINCLE   | UERT0050             |
|        | COMPOTER     | _            |   |                      |
| C      |              |              |   | UERT0060             |
|        | LATEST REVIS | ION -        |   | UERT0070             |
| C      |              |              |   | UERT0080             |
| С      | PURPOSE      | -            | PRINT A MESSAGE REFLECTING AN ERROR CONDITION   | UERT0090             |
| C      |              |              |   | UERT0100             |
| С      | USAGE        | -            | CALL UERTST (IER, NAME)   | UERT0110             |
| Ċ      |              |              |   | UERT0120             |
| C      | ADCIMENTS    | TED -        |   | UERT0130             |
| 2      |              |              | TED _ T. T WUEDE  | TTEDEO 140           |
| C      |              |              | I = 128 IMPLIES TERMINAL ERROR MESSAGE, I = 64 IMPLIES WARNING WITH FIX MESSAGE, I = 32 IMPLIES WARNING MESSAGE. J = ERROR CODE RELEVANT TO CALLING ROUTINE. A CHARACTER STRING OF LENGTH SIX PROVIDING | UERIU140             |
| מממממ  |              |              | 1 = 128 IMPLIES TERMINAL ERROR MESSAGE,   | UERTU150             |
| C      |              |              | I = 64 IMPLIES WARNING WITH FIX MESSAGE,  | UERT0160             |
| C      |              |              | I = 32 IMPLIES WARNING MESSAGE.   | UERT0170             |
| C      |              |              | J = ERROR CODE RELEVANT TO CALLING  | UERT0180             |
| С      |              |              | ROUTINE.  | UERT0190             |
| C      |              | NAME -       | A CHARACTER STRING OF LENGTH SIX PROVIDING  | HERTO200             |
| C      |              |              | THE NAME OF THE CALLING ROUTINE. (INPUT)  | UERT0210             |
|        |              |              | THE NAME OF THE CAUDING ROOTINE. (INFOT)  | UERT0210             |
| C      | /            |              | 07-07-B /3-7-   |                      |
| C      | PRECISION/HA | RDWARE -     |   | UERT0230             |
| C      |              |              |   | UERT0240             |
| С      | REQD. IMSL R | OUTINES -    | - UGETIO, USPKD   | UERT0250<br>UERT0260 |
| С      |              |              |   | UERT0260             |
| С      | NOTATION     | -            | INFORMATION ON SPECIAL NOTATION AND CONVENTIONS IS AVAILABLE IN THE MANUAL  | UERT0270             |
| Č      |              |              | CONVENTIONS IS AVAILABLE IN THE MANUAL  | HERTO280             |
| C      |              |              | INTRODUCTION OR THROUGH IMSL ROUTINE UHELP  |                      |
| ~      |              |              | INTRODUCTION OR THROUGH IMSE ROUTINE UNEELF   | UERT0300             |
| C      |              | mun nano     | D AMOGRAD DOODWARD DV HERMON TO UNITED  |                      |
| C      | REMARKS      |              | R MESSAGE PRODUCED BY UERTST IS WRITTEN   | UERT0310             |
| C      |              |              | TANDARD OUTPUT UNIT. THE OUTPUT UNIT  | UERT0320             |
| C<br>C |              | NUMBER CA    | AN BE DETERMINED BY CALLING UGETIO AS   | UERT0330             |
| C      |              | FOLLOWS.     | . CALL UGETIO (1, NIN, NOUT) .  | UERT0340             |
| C      |              | THE OUTPU    |   | UERT0350             |
| č      |              | TIGETTO A    | S FOLLOWS   | TERT0360             |
| C      |              | COLITO 1.    | NIN - 0   | TERTO370             |
| C      |              |              | NIN = 0 NOUT = NEW OUTPUT UNIT NUMBER CALL UGETIO(3,NIN,NOUT) UGETIO DOCUMENT FOR MORE DETAILS.   | TIEDTO 3 00          |
|        |              |              | NOUT = NEW OUTPUT UNIT NUMBER   | UEKIU300             |
| C      |              |              | CALL UGETIO(3, NIN, NOUT)   | UERTU390             |
| С      |              | SEE THE      | UGETIO DOCUMENT FOR MORE DETAILS.   | UERT0400             |
| С      |              |              | 1982 BY IMSL, INC. ALL RIGHTS RESERVED.  IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN  | UERT0410             |
| С      | COPYRIGHT    | -            | 1982 BY IMSL, INC. ALL RIGHTS RESERVED.   | UERT0420             |
| С      |              |              |   | UERT0430             |
| Ċ      | WARRANTY     | _            | IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN   | UERT0440             |
| C      |              |              |   | UERT0450             |
|        |              |              | EXPRESSED OR IMPLIED, IS APPLICABLE.  | UERT0460             |
| C      |              |              | EXPRESSED OR IMPLIED, IS APPLICABLE.  |                      |
| C      |              |              |   | UERT0470             |
| C      |              |              |   | -UERT0480            |
| С      |              |              |   | UERT0490             |
|        | SUBROUTINE   | UERTST       | (IER, NAME)   | UERT0500             |
| C      |              |              | SPECIFICATIONS FOR ARGUMENTS  | UERT0510             |
|        | INTEGER      |              | IER   | UERT0520             |
|        | INTEGER      |              | NAME (1)  | UERT0530             |
| С      | 1111110111   |              | SPECIFICATIONS FOR LOCAL VARIABLES  | UERT0540             |
| C      | TAMERCED     |              |   |                      |
|        | INTEGER      |              | I, IEQ, IEQDF, IOUNIT, LEVEL, LEVOLD, NAMEQ(6),   | UERT0550             |
|        | *            |              | NAMSET(6), NAMUPK(6), NIN, NMTB   | UERT0560             |
|        | DATA         |              | NAMSET/1HU,1HE,1HR,1HS,1HE,1HT/   | UERT0570             |
|        | DATA         |              | NAMEQ/6*1H /  | UERT0580             |
|        | DATA         |              | LEVEL/4/, IEQDF/0/, IEQ/1H=/  | UERT0590             |
| С      |              |              | UNPACK NAME INTO NAMUPK   | UERT0600             |
| C      |              |              | FIRST EXECUTABLE STATEMENT  | UERT0610             |
| _      | CATT HERVI   | ) (NIXIME) C | , NAMUPK, NMTB)   | UERT0620             |
|        | CMIT OSEVI   | , (IAPITE, 6 | , MARIOT IV, INTID)   | OERI 0620            |

```
GET OUTPUT UNIT NUMBER
                                                                         UERT0630
C
      CALL UGETIO (1, NIN, IOUNIT)
                                                                         UERT0640
                                                                         UERTO650
                                   CHECK IER
C
                                                                         JERT0660
      IF (IER.GT.999) GO TO 25
      IF (IER.LT.-32) GO TO 55
                                                                         UERT0670
      IF (IER.LE.128) GO TO 5
                                                                         UERT0680
      IF (LEVEL.LT.1) GO TO 30
                                                                         UERT0690
                                  PRINT TERMINAL MESSAGE
                                                                        UERT0700
C
      IF (IEQDF.EQ.1) WRITE(IOUNIT, 35) IER, NAMEQ, IEQ, NAMUPK
                                                                        UERT0710
      IF (IEQDF.EQ.0) WRITE (IOUNIT, 35) IER, NAMUPK
                                                                        UERT0720
                                                                         UERT0730
      GO TO 30
    5 IF (IER.LE.64) GO TO 10
                                                                         UERT0740
      IF (LEVEL.LT.2) GO TO 30
                                                                         UERT0750
                                                                      UERT0760
                                  PRINT WARNING WITH FIX MESSAGE
C
      IF (IEQDF.EQ.1) WRITE (IOUNIT, 40) IER, NAMEQ, IEQ, NAMUPK
                                                                         UERT0770
                                                                         UERT0780
      IF (IEQDF.EQ.0) WRITE(IOUNIT,40) IER, NAMUPK
      GO TO 30
                                                                         UERT0790
   10 IF (IER.LE.32) GO TO 15
                                                                         UERT0800
                                   PRINT WARNING MESSAGE
                                                                         UERT0810
C
      IF (LEVEL.LT.3) GO TO 30
                                                                         UERT0820
                                                                        UERT0830
      IF (IEQDF.EQ.1) WRITE (IOUNIT, 45) IER, NAMEQ, IEQ, NAMUPK
      IF (IEODF.EQ.0) WRITE (IOUNIT, 45) IER, NAMUPK
                                                                        UERT0840
      GO TO 30
                                                                         UERT0850
   15 CONTINUE
                                                                         UERT0860
                                   CHECK FOR UERSET CALL
                                                                         UERT0870
                                                                         UERT0880
      DO 20 I=1,6
         IF (NAMUPK(I).NE.NAMSET(I)) GO TO 25
                                                                         UERT0890
   20 CONTINUE
                                                                         UERT0900
      LEVOLD = LEVEL
                                                                         UERT0910
      LEVEL = IER
                                                                         UERT0920
      IER = LEVOLD
                                                                         UERT0930
      IF (LEVEL.LT.0) LEVEL = 4
                                                                         UERT0940
      IF (LEVEL.GT.4) LEVEL = 4
                                                                         UERT0950
      GO TO 30
                                                                         UERT0960
                                                                         UERT0970
   25 CONTINUE
      IF (LEVEL.LT.4) GO TO 30
                                                                        UERT0980
      PRINT NON-DEFINED MESSAGE
IF (IEQDF.EQ.1) WRITE(IOUNIT,50) IER, NAMEQ, IEQ, NAMUPK
                                                                       UERT0990
UERT1000
C
      IF (IEQDF.EQ.0) WRITE(IOUNIT,50) IER, NAMUPK
                                                                        UERT1010
   30 \text{ IEODF} = 0
                                                                         UERT1020
      RETURN
                                                                        UERT1030
   35 FORMAT (19H *** TERMINAL ERROR, 10X, 7H (IER = , I3,
                                                                        UERT1040
     1 20H) FROM IMSL ROUTINE , 6A1, A1, 6A1)
                                                                       UERT1050
   40 FORMAT(27H *** WARNING WITH FIX ERROR, 2X, 7H(IER = , I3,
                                                                        UERT1060
    1 20H) FROM IMSL ROUTINE ,6A1,A1,6A1)
                                                                        UERT1070
   45 FORMAT(18H *** WARNING ERROR, 11X, 7H(IER = , I3,
                                                                        UERT1080
    1 20H) FROM IMSL ROUTINE ,6A1,A1,6A1)
   50 FORMAT(20H *** UNDEFINED ERROR, 9X, 7H(IER = , I5,
                                                                     UERT1110
UERT1120
        20H) FROM IMSL ROUTINE ,6A1,A1,6A1)
                                     P IS THE PAGE NAMUPK
R IS THE POLYMENT
                                   SAVE P FOR P = R CASE
                                                                        UERT1130
                                                                        UERT1140
                                                                        UERT1150
   55 IEQDF = 1
                                                                        UERT1160
      DO 60 I=1,6
                                                                         UERT1170
   60 \text{ NAMEO}(I) = \text{NAMUPK}(I)
                                                                         UERT1180
   65 RETURN
                                                                         UERT1190
      END
                                                                         UERT1200
```

| _     | TMOT DOINGTNE                       | E NAME - UGETIO   | IICEMOO1 O           |  |  |  |
|-------|-------------------------------------|---|----------------------|--|--|--|
| C     | IMSL ROUTINE                        | E NAME - UGETIO   | UGETUUIU             |  |  |  |
| C     |                                     |   | -UGETUUZU            |  |  |  |
| C     |                                     |   | UGET0030             |  |  |  |
| C     | COMPLITTED                          | - IBM/SINGLE  | UGET0050             |  |  |  |
| C     | COMPOTER                            | IBM/SINGEE  | UGET0050             |  |  |  |
| C     | ד.איייבייי סביידי                   | SION - JUNE 1, 1981   | UGET0070             |  |  |  |
| C     | HAILDI KUVIL                        | 3000 17 1901  | UGET0080             |  |  |  |
| C     | PURPOSE                             | - TO RETRIEVE CURRENT VALUES AND TO SET NEW                     | UGET0090             |  |  |  |
| C     | 10111001                            | VALUES FOR INPUT AND OUTPUT UNIT                                | UGET0100             |  |  |  |
| C     |                                     | IDENTIFIERS.  | UGET0110             |  |  |  |
| C     |                                     |   | UGET0120             |  |  |  |
| C     | USAGE                               | - CALL UGETIO (IOPT, NIN, NOUT)                                 | UGET0130             |  |  |  |
| C     |                                     |   | UGET0140             |  |  |  |
| C     | ARGUMENTS                           | IOPT - OPTION PARAMETER. (INPUT)                                | UGET0150             |  |  |  |
| С     |                                     | IF IOPT=1, THE CURRENT INPUT AND OUTPUT                         | UGET0160             |  |  |  |
|       |                                     | UNIT IDENTIFIER VALUES ARE RETURNED IN NIN                      | UGET0170             |  |  |  |
| 00000 |                                     | AND NOUT, RESPECTIVELY.   | UGET0180             |  |  |  |
| С     |                                     | IF IOPT=2, THE INTERNAL VALUE OF NIN IS                         | UGET0190             |  |  |  |
| С     |                                     | RESET FOR SUBSEQUENT USE.                                       | UGET0200             |  |  |  |
| С     |                                     | IF IOPT=3, THE INTERNAL VALUE OF NOUT IS                        | UGET0210             |  |  |  |
| С     |                                     | RESET FOR SUBSEQUENT USE.                                       | UGET0220             |  |  |  |
| С     |                                     | NIN - INPUT UNIT IDENTIFIER.                                    | UGET0230             |  |  |  |
| С     |                                     | NIN - INPUT UNIT IDENTIFIER. OUTPUT IF IOPT=1, INPUT IF IOPT=2. | UGET0240             |  |  |  |
| С     |                                     | NOUT - OUTPUT UNIT IDENTIFIER.                                  | UGET0240<br>UGET0250 |  |  |  |
| С     |                                     | OUTPUT IF IOPT=1, INPUT IF IOPT=3.                              | 00210200             |  |  |  |
| С     |                                     |   | UGET0270             |  |  |  |
| C     | PRECISION/H                         | ARDWARE - SINGLE/ALL  | UGET0280             |  |  |  |
| C     |                                     |   | UGET0290             |  |  |  |
| С     | REQD. IMSL F                        | ROUTINES - NONE REQUIRED  | UGET0300             |  |  |  |
| C     |                                     |   | UGET0310             |  |  |  |
| C     | NOTATION                            | - INFORMATION ON SPECIAL NOTATION AND                           | UGET0320             |  |  |  |
| C     |                                     | CONVENTIONS IS AVAILABLE IN THE MANUAL                          | UGET0330             |  |  |  |
| C     |                                     | INTRODUCTION OR THROUGH IMSL ROUTINE UHELP                      |                      |  |  |  |
| C     | DEMARKO                             | EACH IMSL ROUTINE THAT PERFORMS INPUT AND/OR OUTPUT             | UGET0350             |  |  |  |
| C     | REMARKS                             | OPERATIONS CALLS UGETIO TO OBTAIN THE CURRENT UNIT              | UGET0360<br>UGET0370 |  |  |  |
| C     |                                     | IDENTIFIER VALUES. IF UGETIO IS CALLED WITH IOPT=2 OR           |                      |  |  |  |
| C     |                                     | IOPT=3, NEW UNIT IDENTIFIER VALUES ARE ESTABLISHED.             | UGET0390             |  |  |  |
| C     |                                     | SUBSEQUENT INPUT/OUTPUT IS PERFORMED ON THE NEW UNITS.          |                      |  |  |  |
| C     |                                     | SUBSEQUENT INFOT/OUTFOT IS PERFORMED ON THE NEW UNITS.          | UGET0410             |  |  |  |
| C     | CODVETCHT                           | - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.                       | UGET0410             |  |  |  |
| C     | COFINIOIII                          | 1970 BI INSE, INC. ALE RIGHTS RESERVED.                         | UGET0430             |  |  |  |
| C     | WARRANTY                            | - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN                 |                      |  |  |  |
| C     | WHITE                               | APPLIED TO THIS CODE. NO OTHER WARRANTY,                        | UGET0450             |  |  |  |
| C     |                                     |   | UGET0460             |  |  |  |
| Č     |                                     |   | IICETO470            |  |  |  |
| C     |                                     |   | -UGET0480            |  |  |  |
| C     |                                     |   | UGET0490             |  |  |  |
|       | SUBROUTIN                           | UE UGETIO (IOPT, NIN, NOUT)                                     | UGET0500             |  |  |  |
| С     |                                     | SPECIFICATIONS FOR ARGUMENTS                                    | UGET0510             |  |  |  |
|       | INTEGER                             | IOPT, NIN, NOUT   | UGET0520             |  |  |  |
| С     |                                     | SPECIFICATIONS FOR LOCAL VARIABLES                              | UGET0530             |  |  |  |
|       | INTEGER                             |   | UGET0540             |  |  |  |
|       | DATA                                | NIND/5/, NOUTD/6/   | UGET0550             |  |  |  |
| C     |                                     | FIRST EXECUTABLE STATEMENT                                      | UGET0560             |  |  |  |
|       | IF (IOPT.                           | EQ.3) GO TO 10  | UGET0570             |  |  |  |
|       |                                     |   |                      |  |  |  |
|       | IF (IOPT.                           |   | UGET0580             |  |  |  |
|       | IF (IOPT. IF (IOPT.                 | NE.1) GO TO 9005  | UGET0590             |  |  |  |
|       | IF (IOPT.<br>IF (IOPT.<br>NIN = NIN | NE.1) GO TO 9005  | UGET0590<br>UGET0600 |  |  |  |
|       | IF (IOPT. IF (IOPT.                 | NE.1) GO TO 9005<br>DOUTD                                       | UGET0590             |  |  |  |

5 NIND = NIN
GO TO 9005
10 NOUTD = NOUT
9005 RETURN
END

UGET0630 UGET0640 UGET0650 UGET0660 UGET0670

```
C
   IMSL ROUTINE NAME - USPKD
                                                                    USPK0010
C
                                                                    USPK0020
                        ------USPK0030
C----
                                                                    USPK0040
C
C
   COMPUTER
                      - IBM/SINGLE
                                                                    USPK0050
C
                                                                    USPK0060
C
   LATEST REVISION - NOVEMBER 1, 1984
                                                                    USPK0070
C
                                                                    USPK0080
C
   PURPOSE
                      - NUCLEUS CALLED BY IMSL ROUTINES THAT HAVE
                                                                    USPK0090
C
                         CHARACTER STRING ARGUMENTS
                                                                    USPK0100
C
                                                                    USPK0110
C
   USAGE
                      - CALL USPKD (PACKED, NCHARS, UNPAKD, NCHMTB)
                                                                    USPK0120
C
                                                                    USPK0130
C
   ARGUMENTS PACKED - CHARACTER STRING TO BE UNPACKED. (INPUT)
                                                                    USPK0140
C
               NCHARS - LENGTH OF PACKED. (INPUT) SEE REMARKS.
                                                                    USPK0150
C
              UNPAKD - INTEGER ARRAY TO RECEIVE THE UNPACKED
                                                                    USPK0160
C
                        REPRESENTATION OF THE STRING. (OUTPUT)
                                                                    USPK0170
C
              . NCHMTB - NCHARS MINUS TRAILING BLANKS. (OUTPUT)
                                                                    USPK0180
C
                                                                    USPK0190
C
   PRECISION/HARDWARE - SINGLE/ALL
                                                                    USPK0200
C
                                                                    USPK0210
C
   REOD. IMSL ROUTINES - NONE
                                                                    USPK0220
C
                                                                    USPK0230
C
   REMARKS 1. USPKD UNPACKS A CHARACTER STRING INTO AN INTEGER ARRAY USPK0240
С
               IN (A1) FORMAT.
                                                                    USPK0250
С
            2. UP TO 129 CHARACTERS MAY BE USED. ANY IN EXCESS OF
                                                                    USPK0260
С
               THAT ARE IGNORED.
                                                                    USPK0270
C
                                                                    USPK0280
Ċ
                      - 1984 BY IMSL, INC. ALL RIGHTS RESERVED.
                                                                    USPK0290
C
                                                                    USPK0300
C
   WARRANTY
                     - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN USPK0310
С
                        APPLIED TO THIS CODE. NO OTHER WARRANTY, USPK0320
С
                         EXPRESSED OR IMPLIED, IS APPLICABLE.
                                                                    USPK0330
C
                                                                   USPK0340
C------USPK0350
     SUBROUTINE USPKD (PACKED, NCHARS, UNPAKD, NCHMTB)
                                                                    USPK0360
                               SPECIFICATIONS FOR ARGUMENTS
                                                                    USPK0370
C
                       NC, NCHARS, NCHMTB
                                                                    USPK0380
      INTEGER
C
                                                                    USPK0390
                       UNPAKD(1), PACKED(1), LBYTE, LBLANK
     LOGICAL*1
INTEGER*2
                                                                    USPK0400
                                                                    USPK0410
                       IBYTE, IBLANK
      EQUIVALENCE (LBYTE, IBYTE)
                                                                    USPK0420
                                                                    USPK0430
     DATA
                       LBLANK /1H /
     DATA
                       IBYTE /1H /
                                                                    USPK0440
     DATA
                       IBLANK /1H /
                                                                    USPK0450
C
                                 INITIALIZE NCHMTB
                                                                    USPK0460
     NCHMTB = 0
                                                                    USPK0470
C
                                RETURN IF NCHARS IS LE ZERO
      IF (NCHARS.LE.O) RETURN
C
                                SET NC=NUMBER OF CHARS TO BE DECODED USPK0500
      NC = MINO (129, NCHARS)
                                                                    TISPK0510
      NWORDS = NC*4
                                                                    USPK0520
      J = 1
                                                                    USPK0530
      DO 110 I = 1.NWORDS.4
                                                                    USPK0540
      UNPAKD(I) = PACKED(J)
                                                                    USPK0550
      UNPAKD(I+1) = LBLANK
                                                                    USPK0560
      UNPAKD(I+2) = LBLANK
                                                                    USPK0570
      UNPAKD(I+3) = LBLANK
                                                                    USPK0580
  110 J = J+1
                                                                    USPK0590
C
                                CHECK UNPAKD ARRAY AND SET NCHMTB
                                                                    USPK0600
C
                                BASED ON TRAILING BLANKS FOUND
                                                                    USPK0610
      DO^{\circ}200 N = 1, NWORDS, 4
                                                                    USPK0620
```

| NN = NWORDS - N - 2              | USPK0630 |
|----------------------------------|----------|
| LBYTE = UNPAKD (NN)              | USPK0640 |
| IF (IBYTE .NE. IBLANK) GO TO 210 | USPK0650 |
| 200 CONTINUE                     | USPK0660 |
| NN = 0                           | USPK0670 |
| 210  NCHMTB = (NN + 3) / 4       | USPK0680 |
| RETURN                           | USPK0690 |
| END                              | USPK0700 |
|                                  |          |

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